TABLE A-3-151

CHEMICAL-SPECIFIC INPUTS FOR 4-NITROPHENOL (100-02-7)

Parameter	Reference and Explanation	Equations	Value
Chemical/Physical Properties			
MW (g/mole)	Budavari, O'Neil, Smith, and Heckelman (1989)	--	139.11
T_m (K)	Budavari, O'Neil, Smith, and Heckelman (1989)	--	386.1
Vp (atm)	*Vp* value cited in Howard (1989-1993).	--	1.32E-06 at 25°C (solid)
S (mg/L)	*S* value cited in Howard (1989-1993).	--	2.50E+04
H (atm·m^3/mol)	*H* value was calculated by using the theoretical equation from Lyman, Reehl, and Rosenblatt (1982), which defines the constant. Recommended value was calculated by using the *MW*, *S*, and *Vp* values that are provided in this table.	B-1-6; B-2-6; B-2-8; B-3-6; B-4-6; B-4-12; B-4-19	7.32E-09
D_a (cm^2/s)	D_a value was obtained from CHEMDAT8 database (U.S. EPA 1994d).	B-1-6; B-2-6; B-3-6; B-4-6; B-4-21	4.30E-02
D_w (cm^2/s)	D_w value was obtained from CHEMDAT8 database (U.S. EPA 1994d).	B-4-20	9.61E-06
K_{ow} (unitless)	Arithmetic mean value cited in Karickhoff and Long (1995).	--	8.13E+01
K_{oc} (mL/g)	K_{oc} value was calculated by using the correlation equation with K_{ow} for phthalates and PAHs, / all nonionizing organics except phthalates, PAHs, dioxins, and furans, cited in U.S. EPA (1994c). K_{oc} value was calculated by using the recommended K_{ow} value that is provided in this table.	--	4.37E+02
Kd_s (cm^3/g)	Kd_s value was calculated by using the correlation equation with K_{oc} that is cited in U.S. EPA (1993d) for an assumed organic carbon fraction of 0.01 in soil. Measured organic carbon in soil, specific to site conditions, should be used to calculate Kd_s, because the value varies, depending on the fraction of organic carbon in soil. Recommended Kd_s value was calculated by using the K_{oc} value that is provided in this table.	B-1-3; B-1-4; B-1-5; B-1-6; B-2-3; B-2-4; B-2-5; B-2-6; B-3-3; B-3-4; B-3-5; B-3-6; B-4-3; B-4-4; B-4-5; B-4-6; B-4-10; B-4-11	4.37E+00
Kd_{sw} (L/Kg)	Kd_{sw} value was calculated by using the correlation equation with K_{oc} that is cited in U.S. EPA (1993d) for an assumed organic carbon fraction of 0.075 in suspended sediment. Measured organic carbon in suspended sediment, specific to site conditions, should be used to calculate Kd_{sw}, because the value varies, depending on the fraction of organic carbon in suspended sediment. Recommended Kd_{sw} value was calculated by using the K_{oc} value that is provided in this table.	B-4-16; B-4-18; B-4-24	3.28E+01

TABLE A-3-151

CHEMICAL-SPECIFIC INPUTS FOR 4-NITROPHENOL (100-02-7)

Parameter	Reference and Explanation	Equations	Value
Kd_{bs} (cm^3/g)	Kd_{bs} value was calculated by using the correlation equation with K_{oc} that is cited in U.S. EPA (1993d) for an assumed organic carbon fraction of 0.04 in bottom sediment. Measured organic carbon in bottom sediment, specific to site conditions, should be used to calculate Kd_{bs}, because the value varies, depending on the fraction of organic carbon in bottom sediment. Recommended Kd_{bs} value was calculated by using the K_{oc} value that is provided in this table.	B-4-16; B-4-25	1.75E+01
Chemical/Physical Properties (Continued)			
ksg $(year)^{-1}$	*Ksg* value was calculated by using the chemical half-life in soil, as cited in Howard, Boethling, Jarvis, Meylan, and Michalenko (1991).	B-1-1; B-1-2; B-2-1; B-2-2; B-3-1; B-3-2; B-4-1; B-4-2	2.09E+02
Fv (unitless)	*Fv* value was calculated by using equations cited in Junge (1977) and Bidleman (1988). Recommended value of *Fv* was calculated by using T_m and *Vp* values that are provided in this table. *Vp* value for this compound was converted to a liquid-phase value before being used in the calculations.	B-1-1; B-2-1; B-2-7; B-2-8; B-3-1; B-3-7; B-3-8; B-4-1; B-4-8; B-4-9; B-4-12; B-5-1	1.00
Biotransfer Factors for Plants			
RCF $(\frac{\mu g/g\ DW\ plant}{\mu g/mL\ soil\ water})$	*RCF* value was calculated by using the correlation equation with K_{ow} that is cited in Briggs (1982). Recommended value was calculated by using the K_{ow} value that is provided in this table. The value was then converted to a dry weight basis by using a moisture content of 87 percent.	--	1.32E+01
$Br_{root\ veg}$ $(\frac{\mu g/g\ DW\ plant}{\mu g/g\ soil})$	$Br_{root\ veg}$ value was calculated by dividing the *RCF* value with the Kd_s value provided in this table.	B-2-10	3.01E+00
Br_{ag} $(\frac{\mu g/g\ DW\ plant}{\mu g/g\ soil})$	Br_{ag} value was calculated by using the correlation equation with K_{ow} that is cited in Travis and Arms (1988). No distinction was made between values for aboveground produce and forage. Recommended value was calculated by using the K_{ow} value that is provided in this table.	B-2-9	3.05E+00
Br_{forage} $(\frac{\mu g/g\ DW\ plant}{\mu g/g\ soil})$	Br_{forage} value was calculated by using the correlation equation with K_{ow} that is cited in Travis and Arms (1988). No distinction was made between values for abovegroud produce and forage. Recommended value was calculated by using the K_{ow} value that is provided in this table.	B-3-9	3.05E+00
Bv_{ag} $(\frac{\mu g/g\ DW\ plant}{\mu g/g\ air})$	Bv_{ag} value was calculated by using the correlation equation with K_{ow} and *H* that is cited in Bacci, Calamari, Gaggi, and Vighi (1990); and Bacci, Cerejeira, Gaggi, Chemello, Calamari, and Vighi (1992); then reducing this value by a factor of 100. No distinction was made between values for aboveground produce and forage. Recommended value was calculated, for a temperature (T) of 25°C, by using the *H* and K_{ow} values that are provided in this table.	B-2-8	8.26E+02

TABLE A-3-151

CHEMICAL-SPECIFIC INPUTS FOR 4-NITROPHENOL (100-02-7)

Parameter	Reference and Explanation	Equations	Value
Bv_{forage} ($\frac{\mu g/g\ DW\ plant}{\mu g/g\ air}$)	Bv_{forage} value was calculated by using the correlation equation with K_{ow} and H that is cited in Bacci, Calamari, Gaggi, and Vighi (1990); and Bacci, Cerejeira, Gaggi, Chemello, Calamari, and Vighi (1992); then reducing this value by a factor of 100. No distinction was made between values for aboveground produce and forage. Recommended value was calculated, for a temperature (T) of 25°C, by using the H and K_{ow} values that are provided in this table.	B-3-8	8.26E+02
Biotransfer Factors for Animals			
Ba_{milk} (day/kg FW)	Ba_{milk} value was calculated by using the correlation equation with K_{ow} that is cited in Travis and Arms (1988). Recommended value was calculated by using the K_{ow} value that is provided in this table.	B-3-11	6.46E-07
Ba_{beef} (day/kg FW)	Ba_{beef} value was calculated by using the correlation equation with K_{ow} that is cited in Travis and Arms (1988). Recommended value was calculated by using the K_{ow} value that is provided in this table.	B-3-10	2.04E-06
Ba_{pork} (day/kg FW)	Ba_{pork} value was calculated by using the fat content ratio of pork to beef (23/19) and multiplying it with the Ba_{beef} value.	B-3-12	2.47E-06
Ba_{eggs} (day/kg FW)	Ba_{eggs} value was calculated by using the correlation equation with K_{ow} that is cited in California EPA (1993). Recommended value was calculated by using the K_{ow} value that is provided in this table.	B-3-13	6.46E-04
$Ba_{chicken}$ (day/kg FW)	$Ba_{chicken}$ value was calculated by using the fat content ratio of chicken to beef (15/19) and multiplying it with the Ba_{beef} value.	B-3-14	1.61E-06
BCF_{fish} (L/kg FW tissue)	*BCFs* were used for compounds with a log K_{ow} value below 4.0, as cited in U.S. EPA (1995b). BCF_{fish} value calculated using the correlation equation with K_{ow} obtained from Veith, Macek, Petrocelli, and Caroll (1980)—See Appendix A-3.	B-4-26	1.67E+01
BAF_{fish} (L/kg FW)	--	B-4-27	NA
$BSAF_{fish}$ (unitless)	--	B-4-28	NA
Health Benchmarks			
RfD (mg/kg/day)	U.S. EPA (1997a)	C-1-8	6.20E-02
Oral CSF $(mg/kg/day)^{-1}$	--	C-1-7	NA
RfC (mg/m^3)	Calculated from *RfD* using an inhalation rate of 20 m^3/day and a human body weight of 70 kg.	C-2-3	2.17E-01
Inhalation URF $(\mu g/m^3)^{-1}$	--	C-2-1	NA
Inhalation CSF $(mg/kg/day)^{-1}$	--	C-2-2	NA

Note:

NA = Not applicable
ND = No data available

TABLE A-3-151

CHEMICAL-SPECIFIC INPUTS FOR 4-NITROPHENOL (100-02-7)

All parameters are defined in list of FATE AND TRANSPORT PARAMETERS on page A-3-iii.

TABLE A-3-152

CHEMICAL-SPECIFIC INPUTS FOR N-NITROSO-DI-N-BUTYLAMINE (924-16-3)

Parameter	Reference and Explanation	Equations	Value
Chemical/Physical Properties			
MW (g/mole)	*MW* value cited in U.S. EPA (1995b)	--	158.20
T_m (K)	--	--	NA
Vp (atm)	*Vp* value cited in U.S. EPA (1995b)	--	3.80E-04 at 25°C
S (mg/L)	*S* value cited in U.S. EPA (1995b)	--	1.10E+03
H (atm·m^3/mol)	*H* value was calculated by using the theoretical equation from Lyman, Reehl, and Rosenblatt (1982), which defines the constant. Recommended value was calculated by using the *MW*, *S*, and *Vp* values that are provided in this table.	B-1-6; B-2-6; B-2-8; B-3-6; B-4-6; B-4-12; B-4-19	5.47E-05
D_a (cm^2/s)	D_a value was calculated using the equation cited in U.S. EPA (1996a).	B-1-6; B-2-6; B-3-6; B-4-6; B-4-21	6.50E-02
D_w (cm^2/s)	D_w value was calculated using the equation cited in U.S. EPA (1996a).	B-4-20	7.52E-06
K_{ow} (unitless)	Arithmetic mean value cited in Karickhoff and Long (1995)	--	2.57E+02
K_{oc} (mL/g)	K_{oc} value was calculated by using the correlation equation with K_{ow} for all nonionizing organics except phthalates, PAHs, dioxins, and furans, cited in U.S. EPA (1994c). K_{oc} value was calculated by using the recommended K_{ow} value that is provided in this table.	--	1.07E+02
Kd_s (cm^3/g)	Kd_s value was calculated by using the correlation equation with K_{oc} that is cited in U.S. EPA (1993d) for an assumed organic carbon fraction of 0.01 in soil. Measured organic carbon in soil, specific to site conditions, should be used to calculate Kd_s, because the value varies, depending on the fraction of organic carbon in soil. Recommended Kd_s value was calculated by using the K_{oc} value that is provided in this table.	B-1-3; B-1-4; B-1-5; B-1-6; B-2-3; B-2-4; B-2-5; B-2-6; B-2-10;B-3-3; B-3-4; B-3-5; B-3-6;B-4-3; B-4-4; B-4-5; B-4-6; B-4-10; B-4-11	1.07E+00
Kd_{sw} (L/Kg)	Kd_{sw} value was calculated by using the correlation equation with K_{oc} that is cited in U.S. EPA (1993d) for an assumed organic carbon fraction of 0.075 in suspended sediment. Measured organic carbon in suspended sediment, specific to site conditions, should be used to calculate Kd_{sw}, because the value varies, depending on the fraction of organic carbon in suspended sediment. Recommended Kd_{sw} value was calculated by using the K_{oc} value that is provided in this table.	B-4-16; B-4-18; B-4-24	8.05E+00
Kd_{bs} (cm^3/g)	Kd_{bs} value was calculated by using the correlation equation with K_{oc} that is cited in U.S. EPA (1993d) for an assumed organic carbon fraction of 0.04 in bottom sediment. Measured organic carbon in bottom sediment, specific to site conditions, should be used to calculate Kd_{bs}, because the value varies, depending on the fraction of organic carbon in bottom sediment. Recommended Kd_{bs} value was calculated by using the K_{oc} value that is provided in this table.	B-4-16; B-4-25	4.29E+00

TABLE A-3-152

CHEMICAL-SPECIFIC INPUTS FOR N-NITROSO-DI-N-BUTYLAMINE (924-16-3)

Parameter	Reference and Explanation	Equations	Value
Chemical/Physical Properties (Continued)			
ksg $(year)^{-1}$	*Ksg* value was calculated by using the chemical half-life in soil, as cited in Howard, Boethling, Jarvis, Meylan, and Michalenko (1991).	B-1-2; B-2-2; B-3-2; B-4-2	7.44E+00
Fv (unitless)	*Fv* value cited in NC DEHNR (1997).	B-1-1; B-2-1; B-2-7; B-2-8; B-3-1; B-3-7; B-3-8; B-4-1; B-4-8; B-4-9; B-4-12; B-5-1	1.0
Biotransfer Factors for Plants			
RCF $(\frac{\mu g/g\ DW\ plant}{\mu g/mL\ soil\ water})$	*RCF* value was calculated by using the correlation equation with K_{ow} that is cited in Briggs (1982). Recommended value was calculated by using the K_{ow} value that is provided in this table. The value was then converted to a dry weight basis by using a moisture content of 87 percent.	B-2-10	2.30E+01
$Br_{rootveg}$ $(\frac{\mu g/g\ DW\ plant}{\mu g/g\ soil})$	$Br_{rootveg}$ value was calculated by dividing the *RCF* value with the Kd_s value provided in this table.	B-2-10	2.14E+01
Br_{ag} $(\frac{\mu g/g\ DW\ plant}{\mu g/g\ soil})$	Br_{ag} value was calculated by using the correlation equation with K_{ow} that is cited in Travis and Arms (1988). No distinction was made between values for aboveground produce and forage. Recommended value was calculated by using the K_{ow} value that is provided in this table.	B-2-9	1.57E+00
Br_{forage} $(\frac{\mu g/g\ DW\ plant}{\mu g/g\ soil})$	Br_{forage} value was calculated by using the correlation equation with K_{ow} that is cited in Travis and Arms (1988). No distinction was made between values for aboveground produce and forage. Recommended value was calculated by using the K_{ow} value that is provided in this table.	B-3-9	1.57E+00
Bv_{ag} $(\frac{\mu g/g\ DW\ plant}{\mu g/g\ air})$	Bv_{ag} value was calculated by using the correlation equation with K_{ow} and *H* that is cited in Bacci, Calamari, Gaggi, and Vighi (1990); and Bacci, Cerejeira, Gaggi, Chemello, Calamari, and Vighi (1992); then reducing this value by a factor of 100. No distinction was made between values for aboveground produce and forage. Recommended value was calculated, for a temperature (T) of 25°C, by using the *H* and K_{ow} values that are provided in this table.	B-2-8	3.77E-01
Bv_{forage} $(\frac{\mu g/g\ DW\ plant}{\mu g/g\ air})$	Bv_{forage} value was calculated by using the correlation equation with K_{ow} and *H* that is cited in Bacci, Calamari, Gaggi, and Vighi (1990); and Bacci, Cerejeira, Gaggi, Chemello, Calamari, and Vighi (1992); then reducing this value by a factor of 100. No distinction was made between values for aboveground produce and forage. Recommended value was calculated, for a temperature (T) of 25°C, by using the *H* and K_{ow} values that are provided in this table.	B-3-8	3.77E-01

TABLE A-3-152

CHEMICAL-SPECIFIC INPUTS FOR N-NITROSO-DI-N-BUTYLAMINE (924-16-3)

Parameter	Reference and Explanation	Equations	Value
Biotransfer Factors for Animals			
Ba_{milk} (day/kg FW)	Ba_{milk} value was calculated by using the correlation equation with K_{ow} that is cited in Travis and Arms (1988). Recommended value was calculated by using the K_{ow} value that is provided in this table.	B-3-11	2.04E-06
Ba_{beef} (day/kg FW)	Ba_{beef} value was calculated by using the correlation equation with K_{ow} that is cited in Travis and Arms (1988). Recommended value was calculated by using the K_{ow} value that is provided in this table.	B-3-10	6.46E-06
Ba_{pork} (day/kg FW)	Ba_{pork} value was calculated by using thethe fat content ratio of pork to beef (23/19) and multiplying it with the Ba_{beef} value.	B-3-12	7.82E-06
Ba_{eggs} (day/kg FW)	Ba_{eggs} value was calculated by using the correlation equation with K_{ow} that is cited in California EPA (1993). Recommended value was calculated by using the K_{ow} value that is provided in this table.	B-3-13	2.04E-03
$Ba_{chicken}$ (day/kg FW)	$Ba_{chicken}$ value was calculated by using the fat content ratio of chicken to beef (15/19) and multiplying it with the Ba_{beef} value.	B-3-14	5.10E-06
BCF_{fish} (L/kg FW tissue)	*BCFs* were used for compounds with a log K_{ow} value below 4.0, as cited in U.S. EPA (1995b). BCF_{fish} value calculated using the correlation equation with K_{ow} obtained from Veith, Macek, Petrocelli, and Caroll (1980)—See Appendix A-3.	B-4-26	4.00E+01
BAF_{fish} (L/kg FW)	--	B-4-27	NA
$BSAF_{fish}$ (unitless)	--	B-4-28	NA
Health Benchmarks			
RfD (mg/kg/day)	--	C-1-8	ND
Oral CSF $(mg/kg/day)^{-1}$	U.S. EPA (1997b)	C-1-7	5.4E+00
RfC (mg/m^3)	--	C-2-3	ND
Inhalation URF $(\mu g/m^3)^{-1}$	U.S. EPA (1997b)	C-2-1	1.6E-03
Inhalation CSF $(mg/kg/day)^{-1}$	U.S. EPA (1997c)	C-2-2	5.4E+00

Note:

NA = Not applicable
ND = No data available

All parameters are defined in list of FATE AND TRANSPORT PARAMETERS on page A-3-iii.

TABLE A-3-153

CHEMICAL-SPECIFIC INPUTS FOR *N*-NITROSODIPHENYLAMINE (86-30-6)

Parameter	Reference and Explanation	Equations	Value
Chemical/Physical Properties			
MW (g/mole)	Montgomery and Welkom (1991)	--	198.23
T_m (K)	Montgomery and Welkom (1991)	--	339.6
Vp (atm)	*Vp* value cited in U.S. EPA (1992a).	--	1.74E-07 at 25°C (solid)
S (mg/L)	*S* value cited in U.S. EPA (1992a).	--	3.50E+01
H (atm·m^3/mol)	*H* value was calculated by using the theoretical equation from Lyman, Reehl, and Rosenblatt (1982), which defines the constant. Recommended value was calculated by using the *MW*, *S*, and *Vp* values that are provided in this table.	B-1-6; B-2-6; B-2-8; B-3-6; B-4-6; B-4-12; B-4-19	9.84E-07
D_a (cm^2/s)	D_a value was obtained from CHEMDAT8 database (U.S. EPA 1994d).	B-1-6; B-2-6; B-3-6; B-4-6; B-4-21	3.12E-02
D_w (cm^2/s)	D_w value was obtained from CHEMDAT8 database (U.S. EPA 1994d).	B-4-20	6.35E-06
K_{ow} (unitless)	Geometric mean value cited in U.S. EPA (1994c).	--	1.06E+03
K_{oc} (mL/g)	Estimated value was obtained from U.S. EPA (1994c).	--	3.27E+02, for pH range of 4.9 to 8.0
Kd_s (cm^3/g)	Kd_s value was calculated by using the correlation equation with K_{oc} that is cited in U.S. EPA (1993d) for an assumed organic carbon fraction of 0.01 in soil. Measured organic carbon in soil, specific to site conditions, should be used to calculate Kd_s, because the value varies, depending on the fraction of organic carbon in soil. Recommended Kd_s value was calculated by using the K_{oc} value that is provided in this table.	B-1-3; B-1-4; B-1-5; B-1-6; B-2-3; B-2-4; B-2-5; B-2-6; B-2-10; B-3-3; B-3-4; B-3-5; B-3-6; B-4-3; B-4-4; B-4-5; B-4-6; B-4-10; B-4-11	3.27E+00
Kd_{sw} (L/Kg)	Kd_{sw} value was calculated by using the correlation equation with K_{oc} that is cited in U.S. EPA (1993d) for an assumed organic carbon fraction of 0.075 in suspended sediment. Measured organic carbon in suspended sediment, specific to site conditions, should be used to calculate Kd_{sw}, because the value varies, depending on the fraction of organic carbon in suspended sediment. Recommended Kd_{sw} value was calculated by using the K_{oc} value that is provided in this table.	B-4-16; B-4-18; B-4-24	2.45E+01
Kd_{bs} (cm^3/g)	Kd_{bs} value was calculated by using the correlation equation with K_{oc} that is cited in U.S. EPA (1993d) for an assumed organic carbon fraction of 0.04 in bottom sediment. Measured organic carbon in bottom sediment, specific to site conditions, should be used to calculate Kd_{bs}, because the value varies, depending on the fraction of organic carbon in bottom sediment. Recommended Kd_{bs} value was calculated by using the K_{oc} value that is provided in this table.	B-4-16; B-4-25	1.31E+01

TABLE A-3-153

CHEMICAL-SPECIFIC INPUTS FOR *N*-NITROSODIPHENYLAMINE (86-30-6)

Parameter	Reference and Explanation	Equations	Value
Chemical/Physical Properties (Continued)			
ksg $(year)^{-1}$	*Ksg* value was calculated by using the chemical half-life in soil, as cited in Howard, Boethling, Jarvis, Meylan, and Michalenko (1991).	B-1-2; B-2-2; B-3-2; B-4-2	7.44E+00
Fv (unitless)	*Fv* value was calculated by using equations cited in Junge (1977) and Bidleman (1988). Recommended value of *Fv* was calculated by using T_m and *Vp* values that are provided in this table. *Vp* value for this compound was converted to a liquid-phase value before being used in the calculations.	B-1-1; B-2-1; B-2-7; B-2-8; B-3-1; B-3-7; B-3-8; B-4-1; B-4-8; B-4-9; B-4-12; B-5-1	0.999
Biotransfer Factors for Plants			
RCF $(\frac{\mu g/g\ DW\ plant}{\mu g/mL\ soil\ water})$	*RCF* value was calculated by using the correlation equation with K_{ow} that is cited in Briggs (1982). Recommended value was calculated by using the K_{ow} value that is provided in this table. The value was then converted to a dry weight basis by using a moisture content of 87 percent.	B-2-10	5.61E+01
$Br_{root\ veg}$ $(\frac{\mu g/g\ DW\ plant}{\mu g/g\ soil})$	$Br_{root\ veg}$ value was calculated by dividing the *RCF* value with the Kd_s value provided in this table.	B-2-10	1.71E+01
Br_{ag} $(\frac{\mu g/g\ DW\ plant}{\mu g/g\ soil})$	Br_{ag} value was calculated by using the correlation equation with K_{ow} that is cited in Travis and Arms (1988). No distinction was made between values for aboveground produce and forage. Recommended value was calculated by using the K_{ow} value that is provided in this table.	B-2-9	6.89E-01
Br_{forage} $(\frac{\mu g/g\ DW\ plant}{\mu g/g\ soil})$	Br_{forage} value was calculated by using the correlation equation with K_{ow} that is cited in Travis and Arms (1988). No distinction was made between values for aboveground produce and forage. Recommended value was calculated by using the K_{ow} value that is provided in this table.	B-3-9	6.89E-01
Bv_{ag} $(\frac{\mu g/g\ DW\ plant}{\mu g/g\ air})$	Bv_{ag} value was calculated by using the correlation equation with K_{ow} and *H* that is cited in Bacci, Calamari, Gaggi, and Vighi (1990); and Bacci, Cerejeira, Gaggi, Chemello, Calamari, and Vighi (1992); then reducing this value by a factor of 100. No distinction was made between values foraboveground produce and forage. Recommended value was calculated, for a temperature (T) of 25ºC, by using the *H* and K_{ow} values that are provided in this table.	B-2-8	9.51E+01
Bv_{forage} $(\frac{\mu g/g\ DW\ plant}{\mu g/g\ air})$	Bv_{forage} value was calculated by using the correlation equation with K_{ow} and *H* that is cited in Bacci, Calamari, Gaggi, and Vighi (1990); and Bacci, Cerejeira, Gaggi, Chemello, Calamari, and Vighi (1992); then reducing this value by a factor of 100. No distinction was made between values for aboveground produce and forage. Recommended value was calculated, for a temperature (T) of 25ºC, by using the *H* and K_{ow} values that are provided in this table.	B-3-8	9.51E+01

TABLE A-3-153

CHEMICAL-SPECIFIC INPUTS FOR *N*-NITROSODIPHENYLAMINE (86-30-6)

Parameter	Reference and Explanation	Equations	Value
Biotransfer Factors for Animals			
Ba_{milk} (day/kg FW)	Ba_{milk} value was calculated by using the correlation equation with K_{ow} that is cited in Travis and Arms (1988). Recommended value was calculated by using the K_{ow} value that is provided in this table.	B-3-11	8.45E-06
Ba_{beef} (day/kg FW)	Ba_{beef} value was calculated by using the correlation equation with K_{ow} that is cited in Travis and Arms (1988). Recommended value was calculated by using the K_{ow} value that is provided in this table.	B-3-10	2.67E-05
Ba_{pork} (day/kg FW)	Ba_{pork} value was calculated by using the fat content ratio of pork to beef (23/19) and multiplying it with the Ba_{beef} value.	B-3-12	3.24E-05
Ba_{egg} (day/kg FW)	Ba_{egg} value was calculated by using the correlation equation with K_{ow} that is cited in California EPA (1993). Recommended value was calculated by using the K_{ow} value that is provided in this table.	B-3-13	8.45E-03
$Ba_{chicken}$ (day/kg FW)	$Ba_{chicken}$ value was calculated by using the fat content ratio of chicken to beef (15/19) and multiplying it with the Ba_{beef} value.	B-3-14	2.11E-05
BCF_{fish} (L/kg FW tissue)	*BCFs* were used for compounds with a log K_{ow} value below 4.0, as cited in U.S. EPA (1995b). BCF_{fish} value calculated using the correlation equation with K_{ow} obtained from Veith, Macek, Petrocelli, and Caroll (1980)—See Appendix A-3.	B-4-26	1.18E+02
BAF_{fish} (L/kg, FW)	--	B-4-27	NA
$BSAF_{fish}$ (unitless)	--	B-4-28	NA
Health Benchmarks			
RfD (mg/kg/day)	--	C-1-8	ND
Oral CSF $(mg/kg/day)^{-1}$	U.S.EPA (1997b)	C-1-7	4.9E-03
RfC (mg/m^3)	--	C-2-3	ND
Inhalation URF $(\mu g/m^3)^{-1}$	Calculated from *Oral CSF* using an inhalation rate of 20 m^3/day and a human body weight of 70 kg.	C-2-1	1.4E-06
Inhalation CSF $(mg/kg/day)^{-1}$	Value based on *Oral CSF* assuming route-to-route extrapolation.	C-2-2	4.9E-03

Note:

NA = Not applicable
ND = No data available

All parameters are defined in list of FATE AND TRANSPORT PARAMETERS on page A-3-iii.

TABLE A-3-154

CHEMICAL-SPECIFIC INPUTS FOR *N*-NITROSODIPROPYLAMINE (621-64-7)

Parameter	Reference and Explanation	Equations	Value
Chemical/Physical Properties			
MW (g/mole)	Montgomery and Welkom (1991)	--	130.19
T_m (K)	--	--	ND
Vp (atm)	Geometric mean value cited in U.S. EPA (1992a).	--	6.09E-06 at 25°C (liquid)
S (mg/L)	Geometric mean value cited in U.S. EPA (1992a).	--	1.46E+04
H (atm·m^3/mol)	*H* value was calculated by using the theoretical equation from Lyman, Reehl, and Rosenblatt (1982), which defines the constant. Recommended value was calculated by using the *MW*, *S*, and *Vp* values that are provided in this table.	B-1-6; B-2-6; B-2-8; B-3-6; B-4-6; B-4-12; B-4-19	5.43E-08
D_a (cm^2/s)	D_a value was obtained from CHEMDAT8 database (U.S. EPA 1994d).	B-1-6; B-2-6; B-3-6; B-4-6; B-4-21	5.67E-02
D_w (cm^2/s)	D_w value was obtained from CHEMDAT8 database (U.S. EPA 1994d).	B-4-20	7.75E-06
K_{ow} (unitless)	K_{ow} value cited in U.S. EPA (1995b).	--	2.40E+01
K_{oc} (mL/g)	K_{oc} value was calculated by using the correlation equation with K_{ow} for phthalates and PAHs, / all nonionizing organics except phthalates, PAHs, dioxins, and furans, cited in U.S. EPA (1994c). K_{oc} value was calculated by using the recommended K_{ow} value that is provided in this table.	--	1.70E+01
Kd_s (cm^3/g)	Kd_s value was calculated by using the correlation equation with K_{oc} that is cited in U.S. EPA (1993d) for an assumed organic carbon fraction of 0.01 in soil. Measured organic carbon in soil, specific to site conditions, should be used to calculate Kd_s, because the value varies, depending on the fraction of organic carbon in soil. Recommended Kd_s value was calculated by using the K_{oc} value that is provided in this table.	B-1-3; B-1-4; B-1-5; B-1-6; B-2-3; B-2-4; B-2-5; B-2-6; B-2-10; B-3-3; B-3-4; B-3-5; B-3-6; B-4-3; B-4-4; B-4-5; B-4-6; B-4-10; B-4-11	1.70E-01
Kd_{sw} (L/Kg)	Kd_{sw} value was calculated by using the correlation equation with K_{oc} that is cited in U.S. EPA (1993d) for an assumed organic carbon fraction of 0.075 in suspended sediment. Measured organic carbon in suspended sediment, specific to site conditions, should be used to calculate Kd_{sw}, because the value varies, depending on the fraction of organic carbon in suspended sediment. Recommended Kd_{sw} value was calculated by using the K_{oc} value that is provided in this table.	B-4-16; B-4-18; B-4-24	1.28E+00

TABLE A-3-154

CHEMICAL-SPECIFIC INPUTS FOR *N*-NITROSODIPROPYLAMINE (621-64-7)

Parameter	Reference and Explanation	Equations	Value
Chemical/Physical Properties (Continued)			
Kd_{bs} (cm^3/g)	Kd_{bs} value was calculated by using the correlation equation with K_{oc} that is cited in U.S. EPA (1993d) for an assumed organic carbon fraction of 0.04 in bottom sediment. Measured organic carbon in bottom sediment, specific to site conditions, should be used to calculate Kd_{bs}, because the value varies, depending on the fraction of organic carbon in bottom sediment. Recommended Kd_{bs} value was calculated by using the K_{oc} value that is provided in this table.	B-4-16; B-4-25	6.80E-01
ksg $(year)^{-1}$	*Ksg* value was calculated by using the chemical half-life in soil, as cited in Howard, Boethling, Jarvis, Meylan, and Michalenko (1991)	B-1-1; B-1-2; B-2-1; B-2-2; B-3-1; B-3-2; B-4-1; B-4-2	1.41E+00
Fv (unitless)	*Fv* value was calculated by using the equation cited in Junge (1977). Recommended value of *Fv* was calculated by using the *Vp* value that is provided in the table.	B-1-1; B-2-1; B-2-7; B-2-8; B-3-1; B-3-7; B-3-8; B-4-1; B-4-8; B-4-9; B-4-12; B-5-1	1.00
Biotransfer Factors for Plants			
RCF $(\frac{\mu g/g\ DW\ plant}{\mu g/mL\ soil\ water})$	*RCF* value was calculated by using the correlation equation with K_{ow} that is cited in Briggs (1982). Recommended value was calculated by using the K_{ow} value that is provided in this table. The value was then converted to a dry weight basis by using a moisture content of 87 percent.	B-2-10	8.99E+00
$Br_{rootveg}$ $(\frac{\mu g/g\ DW\ plant}{\mu g/g\ soil})$	$Br_{rootveg}$ value was calculated by dividing the *RCF* value with the Kd_s value provided in this table.	B-2-10	5.29E+01
Br_{ag} $(\frac{\mu g/g\ DW\ plant}{\mu g/g\ soil})$	Br_{ag} value was calculated by using the correlation equation with K_{ow} that is cited in Travis and Arms (1988). No distinction was made between values for aboveground produce and forage. Recommended value was calculated by using the K_{ow} value that is provided in this table.	B-2-9	6.17E+00
Br_{forage} $(\frac{\mu g/g\ DW\ plant}{\mu g/g\ soil})$	Br_{forage} value was calculated by using the correlation equation with K_{ow} that is cited in Travis and Arms (1988). No distinction was made between values for aboveground produce and forage. Recommended value was calculated by using the K_{ow} value that is provided in this table.	B-3-9	6.17E+00
Bv_{ag} $(\frac{\mu g/g\ DW\ plant}{\mu g/g\ air})$	Bv_{ag} value was calculated by using the correlation equation with K_{ow} and *H* that is cited in Bacci, Calamari, Gaggi, and Vighi (1990); and Bacci, Cerejeira, Gaggi, Chemello, Calamari, and Vighi (1992); then reducing this value by a factor of 100. No distinction was made between values for aboveground produce and forage. Recommended value was calculated, for a temperature (T) of 25°C, by using the *H* and K_{ow} values that are provided in this table.	B-2-8	3.04E+01

TABLE A-3-154

CHEMICAL-SPECIFIC INPUTS FOR *N*-NITROSODIPROPYLAMINE (621-64-7)

Parameter	Reference and Explanation	Equations	Value
Biotransfer Factors for Plants (continued)			
Bv_{forage} $(\frac{\mu g/g\ DW\ plant}{\mu g/g\ air})$	Bv_{forage} value was calculated by using the correlation equation with K_{ow} and H that is cited in Bacci, Calamari, Gaggi, and Vighi (1990); and Bacci, Cerejeira, Gaggi, Chemello, Calamari, and Vighi (1992); then reducing this value by a factor of 100. No distinction was made between values for aboveground produce and forage. Recommended value was calculated, for a temperature (T) of 25°C, by using the H and K_{ow} values that are provided in this table.	B-3-8	3.04E+01
Biotransfer Factors for Animals			
Ba_{milk} (day/kg FW)	Ba_{milk} value was calculated by using the correlation equation with K_{ow} that is cited in Travis and Arms (1988). Recommended value was calculated by using the K_{ow} value that is provided in this table.	B-3-11	1.91E-07
Ba_{beef} (day/kg FW)	Ba_{beef} value was calculated by using the correlation equation with K_{ow} that is cited in Travis and Arms (1988). Recommended value was calculated by using the K_{ow} value that is provided in this table.	B-3-10	6.03E-07
Ba_{pork} (day/kg FW)	Ba_{pork} value was calculated by using the fat content ratio of pork to beef (23/19) and multiplying it with the Ba_{beef} value.	B-3-12	7.30E-07
Ba_{egg} (day/kg FW)	Ba_{egg} value was calculated by using the correlation equation with K_{ow} that is cited in California EPA (1993). Recommended value was calculated by using the K_{ow} value that is provided in this table.	B-3-13	1.91E-04
$Ba_{chicken}$ (day/kg FW)	$Ba_{chicken}$ value was calculated by using the fat content ratio of chicken to beef (15/19) and multiplying it with the Ba_{beef} value.	B-3-14	4.76E-07
BCF_{fish} (L/kg FW tissue)	*BCFs* were used for compounds with a log K_{ow} value below 4.0, as cited in U.S. EPA (1995b). BCF_{fish} value calculated using the correlation equation with K_{ow} obtained from Veith, Macek, Petrocelli, and Caroll (1980)—See Appendix A-3.	B-4-26	6.59E+00
BAF_{fish} (L/kg FW)	--	B-4-27	NA
$BSAF_{fish}$ (unitless)	--	B-4-28	NA
Health Benchmarks			
RfD (mg/kg/day)		C-1-8	ND
Oral CSF $(mg/kg/day)^{-1}$	U.S. EPA (1997b)	C-1-7	7.0E+00
RfC (mg/m^3)		C-2-3	ND
Inhalation URF $(\mu g/m^3)^{-1}$	U.S. EPA (1997b)	C-2-1	2.0E-03
Inhalation CSF $(mg/kg/day)^{-1}$	U.S. EPA (1997b)	C-2-2	7.0E+00

Note:

NA = Not applicable

TABLE A-3-154

CHEMICAL-SPECIFIC INPUTS FOR *N*-NITROSODIPROPYLAMINE (621-64-7)

ND = No data available
All parameters are defined in list of FATE AND TRANSPORT PARAMETERS on page A-3-iii.

TABLE A-3-155

CHEMICAL-SPECIFIC INPUTS FOR 1,2,3,4,6,7,8,9-OCTACHLORODIBENZO(P)DIOXIN (3268-87-9)

Parameter	Reference and Explanation	Equations	Value
Chemical/Physical Properties			
MW (g/mole)	U.S. EPA (1994a)	--	460.76
T_m (K)	U.S. EPA (1994a)	--	598.1
Vp (atm)	U.S. EPA (1994a)	--	8.61E-11 at 25°C (solid)
S (mg/L)	U.S. EPA (1994a)	--	4.00E-07
H (atm·m^3/mol)	U.S. EPA (1994a)	B-1-6; B-2-6; B-2-8; B-3-6; B-4-6; B-4-12; B-4-19	7.00E-09
D_a (cm^2/s)	D_a value was obtained from CHEMDAT8 database (U.S. EPA 1994d).	B-1-6; B-2-6; B-3-6; B-4-6; B-4-21	1.06E-02
D_w (cm^2/s)	D_w value was calculated using the equation cited in U.S. EPA (1996a).	B-4-20	3.69E-07
K_{ow} (unitless)	U.S. EPA (1994a)	--	3.89E+07
K_{oc} (mL/g)	K_{oc} value was calculated by using the correlation equation with K_{ow} for dioxins and furans that is cited in U.S. EPA (1994a; 1994c). Recommended value was calculated by using the recommended K_{ow} value that is provided in this table.	--	2.40E+07
Kd_s (cm^3/g)	Kd_s value was calculated by using the correlation equation with K_{oc} that is cited in U.S. EPA (1993d) for an assumed organic carbon fraction of 0.01 in soil. Measured organic carbon in soil, specific to site conditions, should be used to calculate Kd_s, because the value varies, depending on the fraction of organic carbon in soil. Recommended Kd_s value was calculated by using the K_{oc} value that is provided in this table.	B-1-3; B-1-4; B-1-5; B-1-6; B-2-3; B-2-4; B-2-5; B-2-6; B-2-10; B-3-3; B-3-4; B-3-5; B-3-6; B-4-3; B-4-4; B-4-5; B-4-6; B-4-10; B-4-11	2.40E+05
Kd_{sw} (L/Kg)	Kd_{sw} value was calculated by using the correlation equation with K_{oc} that is cited in U.S. EPA (1993d) for an assumed organic carbon fraction of 0.075 in suspended sediment. Measured organic carbon in suspended sediment, specific to site conditions, should be used to calculate Kd_{sw}, because the value varies, depending on the fraction of organic carbon in suspended sediment. Recommended Kd_{sw} value was calculated by using the K_{oc} value that is provided in this table.	B-4-16; B-4-18; B-4-24	1.80E+06

TABLE A-3-155

CHEMICAL-SPECIFIC INPUTS FOR 1,2,3,4,6,7,8,9-OCTACHLORODIBENZO(P)DIOXIN (3268-87-9)

Parameter	Reference and Explanation	Equations	Value
Kd_{bs} (cm^3/g)	Kd_{bs} value was calculated by using the correlation equation with K_{oc} that is cited in U.S. EPA (1993d) for an assumed organic carbon fraction of 0.04 in bottom sediment. Measured organic carbon in bottom sediment, specific to site conditions, should be used to calculate Kd_{bs}, because the value varies depending on the fraction of organic carbon in bottom sediment. Recommended Kd_{bs} value was calculated by using the K_{oc} value that is provided in this table.	B-4-16; B-4-25	9.60E+05
Chemical/Physical Properties (Continued)			
ksg $(year)^{-1}$	*ksg* value was calculated by using the chemical half-life in soil, as cited in Mackay, Shiu, and Ma (1992).	B-1-1; B-1-2; B-2-1; B-2-2; B-3-1; B-3-2; B-4-1; B-4-2	1.09E-01
Fv (unitless)	*Fv* value was calculated by using equations cited in Junge (1977) and Bidleman (1988). Recommended value of Fv was calculated by using T_m and *Vp* values that are provided in this table. *Vp* value for this compound was converted to a liquid-phase value before being used in the calculations.	B-1-1; B-2-1; B-2-7; B-2-8; B-3-1; B-3-7; B-3-8; B-4-1; B-4-8; B-4-9; B-4-12; B-5-1	9.93E-01
Biotransfer Factors for Plants			
RCF $(\frac{\mu g/g\ DW\ plant}{\mu g/mL\ soil\ water})$	*RCF* value was calculated by using the correlation equation with K_{ow} that is cited in Briggs (1982). Recommended value was calculated by using the K_{ow} value that is provided in this table. The value was then converted to a dry weight basis by using a moisture content of 87 percent.	B-2-10	1.62E+05
$Br_{root\ veg}$ $(\frac{\mu g/g\ DW\ plant}{\mu g/g\ soil})$	$Br_{root\ veg}$ value was calculated by dividing the *RCF* value with the Kd_s value provided in this table.	B-2-10	6.77E-01
Br_{ag} $(\frac{\mu g/g\ DW\ plant}{\mu g/g\ soil})$	Br_{ag} value was calculated by using the correlation equation with K_{ow} that is cited in Travis and Arms (1988). No distinction was made between values for aboveground produce and forage. Recommended value was calculated by using the K_{ow} value that is provided in this table.	B-2-9	1.59E-03
Br_{forage} $(\frac{\mu g/g\ DW\ plant}{\mu g/g\ soil})$	Br_{forage} value was calculated by using the correlation equation with K_{ow} that is cited in Travis and Arms (1988). No distinction was made between values for aboveground produce and forage. Recommended value was calculated by using the K_{ow} value that is provided in this table.	B-3-9	1.59E-03
Bv_{ag} $(\frac{\mu g/g\ DW\ plant}{\mu g/g\ air})$	Bv_{ag} value was obtained from Lorber (1995). No distinction was made between aboveground produce and forage.	B-2-8	8.60E+06

TABLE A-3-155

CHEMICAL-SPECIFIC INPUTS FOR 1,2,3,4,6,7,8,9-OCTACHLORODIBENZO(P)DIOXIN (3268-87-9)

Parameter	Reference and Explanation	Equations	Value
Bv_{forage} $(\frac{\mu g/g\ DW\ plant}{\mu g/g\ air})$	Bv_{forage} value was obtained from Lorber (1995). No distinction was made between aboveground produce and forage.	B-3-8	8.60E+06
Biotransfer Factors for Animals			
Ba_{milk} (day/kg FW)	U.S. EPA (1995a)	B-3-11	1.00E-03
Ba_{beef} (day/kg FW)	Ba_{beef} value was calculated by increasing Ba_{milk} values by a factor of 5.43, as discussed in Section A3.3.14.	B-3-10	5.43E-03
Biotransfer Factors for Animals (Continued)			
Ba_{pork} (day/kg FW)	Ba_{pork} value was calculated by increasing Ba_{milk} values by a factor of 6.57, as discussed in Section A3.3.15.	B-3-12	6.57E-03
Ba_{egg} (L/kg FW tissue)	Ba_{egg} value was calculated by multiplying the BCF value for chicken eggs by a chicken soil consumption rate of 0.02 kg (DW)/day (See Appendix A-3). BCF value for eggs was obtained from Stephens, Petreas, and Hayward (1995) for the high exposure chicken group.	B-3-13	9.90E-03
$Ba_{chicken}$ (unitless, FW tissue)	$Ba_{chicken}$ value was calculated by multiplying the BCF value for chicken by a chicken soil consumption rate of 0.02 kg (DW)/day (See Appendix A-3). BCF value for chicken was obtained from Stephens, Petreas, and Hayward (1995) for the high exposure chicken group.	B-3-14	1.10E-03
BCF_{fish} (L/kg FW tissue)	--	B-4-26	NA
BAF_{fish} (L/kg FW)	--	B-4-27	NA
$BSAF_{fish}$ (unitless, lipid based)	U.S. EPA (1994a)	B-4-28	1.00E-04
Other Parameters			
TEF (unitless)	U.S. EPA (1994a)	--	0.001
Health Benchmarks			
Oral CSF $(mg/kg/day)^{-1}$	--	C-1-8	ND
Inhalation CSF $(mg/kg/day)^{-1}$	--	C-1-7	ND
RfD (mg/kg/day)	--	C-2-3	ND
Inhalation URF $(\mu g/m^3)^{-1}$	--	C-2-1	ND
RfC (mg/m^3)	--	C-2-2	ND

TABLE A-3-155

CHEMICAL-SPECIFIC INPUTS FOR 1,2,3,4,6,7,8,9-OCTACHLORODIBENZO(P)DIOXIN (3268-87-9)

Note:

NA = Not Applicable; ND = No Data Available
All parameters are defined in list of FATE AND TRANSPORT PARAMETERS on page A-3-iii.

TABLE A-3-156

CHEMICAL-SPECIFIC INPUTS FOR 1,2,3,4,6,7,8,9-OCTACHLORODIBENZO(P)FURAN (39001-02-0)

Parameter	Reference and Explanation	Equations	Value
Chemical/Physical Properties			
MW (g/mole)	U.S. EPA (1994a)	--	444.76
T_m (K)	U.S. EPA (1994a)	--	531.1
Vp (atm)	U.S. EPA (1994a)	--	4.93E-15 at 25°C (solid)
S (mg/L)	U.S. EPA (1994a)	--	1.20E-06
H (atm·m^3/mol)	U.S.EPA (1994a)	B-1-6; B-2-6; B-2-8; B-3-6; B-4-6; B-4-12; B-4-19	1.90E-06
D_a (cm^2/s)	D_a value was obtained from CHEMDAT8 database (U.S. EPA 1994d).	B-1-6; B-2-6; B-3-6; B-4-6; B-4-21	1.48E-02
D_w (cm^2/s)	D_w value was calculated using the equation cited in U.S. EPA (1996a).	B-4-20	3.78E-06
K_{ow} (unitless)	U.S. EPA (1994a)	--	6.03E+08
K_{oc} (mL/g)	K_{oc} value was calculated by using the correlation equation with K_{ow} for dioxins and furans that is cited in U.S. EPA (1994a) and U.S. EPA (1994c). Recommended value was calculated by using the recommended K_{ow} value that is provided in this table.	--	3.72E+08
Kd_s (cm^3/g)	Kd_s value was calculated by using the correlation equation with K_{oc} that is cited in U.S. EPA (1993d) for an assumed organic carbon fraction of 0.01 in soil. Measured organic carbon in soil, specific to site conditions, should be used to calculate Kd_s, because the value varies, depending on the fraction of organic carbon in soil. Recommended Kd_s value was calculated by using the K_{oc} value that is provided in this table.	B-1-3; B-1-4; B-1-5; B-1-6; B-2-3; B-2-4; B-2-5; B-2-6; B-2-10; B-3-3; B-3-4; B-3-5; B-3-6; B-4-3; B-4-4; B-4-5; B-4-6; B-4-10; B-4-11	3.72E+06
Kd_{sw} (L/Kg)	Kd_{sw} value was calculated by using the correlation equation with K_{oc} that is cited in U.S. EPA (1993d) for an assumed organic carbon fraction of 0.075 in suspended sediment. Measured organic carbon in suspended sediment, specific to site conditions, should be used to calculate Kd_{sw}, because the value varies, depending on the fraction of organic carbon in suspended sediment. Recommended Kd_{sw} value was calculated by using the K_{oc} value that is provided in this table.	B-4-16; B-4-18; B-4-24	2.79E+07

TABLE A-3-156

CHEMICAL-SPECIFIC INPUTS FOR 1,2,3,4,6,7,8,9-OCTACHLORODIBENZO(P)FURAN (39001-02-0)

Parameter	Reference and Explanation	Equations	Value
Kd_{bs} (cm^3/g)	Kd_{bs} value was calculated by using the correlation equation with K_{oc} that is cited in U.S. EPA (1993d) for an assumed organic carbon fraction of 0.04 in bottom sediment. Measured organic carbon in bottom sediment, specific to site conditions, should be used to calculate Kd_{bs}, because the value varies depending on the fraction of organic carbon in bottom sediment. Recommended Kd_{bs} value was calculated by using the K_{oc} value that is provided in this table.	B-4-16; B-4-25	1.49E+07
ksg $(year)^{-1}$	*ksg* value was calculated by using the chemical half-life in soil, as cited in Mackay, Shiu, and Ma (1992).	B-1-1; B-1-2; B-2-1; B-2-2; B-3-1; B-3-2; B-4-1; B-4-2	1.10E-01
Fv (unitless)	*Fv* value was calculated by using equations cited in Junge (1977) and Bidleman (1988). Recommended value of Fv was calculated by using T_m and *Vp* values that are provided in this table. *Vp* value for this compound was converted to a liquid phase value before being used in the calculations.	B-1-1; B-2-1; B-2-7; B-2-8; B-3-1; B-3-7; B-3-8; B-4-1; B-4-8; B-4-9; B-4-12; B-5-1	1.67E-03
Biotransfer Factors for Plants			
RCF $(\frac{\mu g/g\ DW\ plant}{\mu g/mL\ soil\ water})$	*RCF* value was calculated by using the correlation equation with K_{ow} that is cited in Briggs (1982). Recommended value was calculated by using the K_{ow} value that is provided in this table. The value was then converted to a dry weight basis by using a moisture content of 87 percent.	B-2-10	1.34E+06
$Br_{rootveg}$ $(\frac{\mu g/g\ DW\ plant}{\mu g/g\ soil})$	$Br_{rootveg}$ value was calculated by dividing the *RCF* value with the Kd_s value provided in this table.	B-2-10	3.60E-01
Br_{ag} $(\frac{\mu g/g\ DW\ plant}{\mu g/g\ soil})$	Br_{ag} value was calculated by using the correlation equation with K_{ow} that is cited in Travis and Arms (1988). No distinction was made between values for aboveground produce and forage. Recommended value was calculated by using the K_{ow} value that is provided in this table.	B-2-9	3.26E-04
Br_{forage} $(\frac{\mu g/g\ DW\ plant}{\mu g/g\ soil})$	Br_{forage} value was calculated by using the correlation equation with K_{ow} that is cited in Travis and Arms (1988). No distinction was made between values for aboveground produce and forage. Recommended value was calculated by using the K_{ow} value that is provided in this table.	B-3-9	3.26E-04
Bv_{ag} $(\frac{\mu g/g\ DW\ plant}{\mu g/g\ air})$	Bv_{ag} value was obtained from Lorber (1995). No distinction was made between aboveground produce and forage.	B-2-8	1.30E+06

TABLE A-3-156

CHEMICAL-SPECIFIC INPUTS FOR 1,2,3,4,6,7,8,9-OCTACHLORODIBENZO(P)FURAN (39001-02-0)

Parameter	Reference and Explanation	Equations	Value
Biotransfer Factors for Plants (Continued)			
Bv_{forage} ($\frac{\mu g/g\ DW\ plant}{\mu g/g\ air}$)	Bv_{forage} value was obtained from Lorber (1995). No distinction was made between aboveground produce and forage.	B-3-8	1.30E+06
Biotransfer Factors for Animals			
Ba_{milk} (day/kg FW)	U.S. EPA (1995a)	B-3-11	1.00E-03
Ba_{beef} (day/kg FW)	Ba_{beef} value was calculated by increasing Ba_{milk} values by a factor of 5.43, as discussed in Section A3.3.14.	B-3-10	5.43E-03
Ba_{pork} (day/kg FW)	Ba_{pork} value was calculated by increasing Ba_{milk} values by a factor of 6.57, as discussed in Section A3.3.15.	B-3-12	6.57E-03
Ba_{egg} (L/kg FW tissue)	Ba_{egg} value was calculated by multiplying the BCF value for chicken eggs by a chicken soil consumption rate of 0.02 kg (DW)/day (See Appendix A-3). BCF value for eggs was obtained from Stephens, Petreas, and Hayward (1995) for the high exposure chicken group.	B-3-13	7.92E-03
$Ba_{chicken}$ (L/kg FW tissue)	$Ba_{chicken}$ value was calculated by multiplying the BCF value for chicken by a chicken soil consumption rate of 0.02 kg (DW)/day (see Appendix A-3). BCF value for chicken was obtained from Stephens, Petreas, and Hayward (1995) for the high exposure chicken group.	B-3-14	4.40E-04
BCF_{fish} (L/kg FW tissue)	--	B-4-26	NA
BAF_{fish} (L/kg FW)	--	B-4-27	NA
$BSAF_{fish}$ (unitless, lipid based)	U.S. EPA (1994a)	B-4-28	1.00E-04
Other Parameters			
TEF (unitless)	U.S. EPA (1994a)	--	0.001
Health Benchmarks			
Oral CSF $(mg/kg/day)^{-1}$	--	C-1-8	ND
Inhalation CSF $(mg/kg/day)^{-1}$	--	C-1-7	ND
RfD (mg/kg/day)	--	C-2-3	ND
Inhalation URF $(\mu g/m^3)^{-1}$	--	C-2-1	ND
RfC (mg/m^3)	--	C-2-2	ND

TABLE A-3-156

CHEMICAL-SPECIFIC INPUTS FOR 1,2,3,4,6,7,8,9-OCTACHLORODIBENZO(P)FURAN (39001-02-0)

Note:

NA = Not Applicable; ND = No Data Available
All parameters are defined in list of FATE AND TRANSPORT PARAMETERS on page A-3-iii.

TABLE A-3-157

CHEMICAL-SPECIFIC INPUTS FOR 1,2,3,7,8-PENTACHLORODIBENZO(P)DIOXIN (40321-76-4)

Parameter	Reference and Explanation	Equations	Value
Chemical/Physical Properties			
MW (g/mole)	U.S. EPA (1994a)	--	356.42
T_m (K)	U.S. EPA (1994a)	--	513.1
Vp (atm)	U.S. EPA (1994a)	--	1.25E-12 at 25°C (solid)
S (mg/L)	Homologue group average value obtained from U.S. EPA (1994a).	--	1.20E-04
H (atm·m^3/mol)	U.S. EPA (1994a)	B-1-6; B-2-6; B-2-8; B-3-6; B-4-6; B-4-12; B-4-19	2.60E-06
D_a (cm^2/s)	D_a value was obtained from CHEMDAT8 database (U.S. EPA 1994d).	B-1-6; B-2-6; B-3-6; B-4-6; B-4-21	1.21E-02
D_w (cm^2/s)	D_w value was calculated using the equation cited in U.S. EPA (1996a).	B-4-20	4.38E-06
K_{ow} (unitless)	U.S. EPA (1992d)	--	4.37E+06
K_{oc} (mL/g)	K_{oc} value was calculated by using the correlation equation with K_{ow} for dioxins and furans that is cited in U.S. EPA (1994a) and U.S. EPA (1994c). Recommended value was calculated by using the recommended K_{ow} value that is provided in this table.	--	2.69E+06
Kd_s (cm^3/g)	Kd_s value was calculated by using the correlation equation with K_{oc} that is cited in U.S. EPA (1993d) for an assumed organic carbon fraction of 0.01 in soil. Measured organic carbon in soil, specific to site conditions, should be used to calculate Kd_s, because the value varies, depending on the fraction of organic carbon in soil. Recommended Kd_s value was calculated by using the K_{oc} value that is provided in this table.	B-1-3; B-1-4; B-1-5; B-1-6; B-2-3; B-2-4; B-2-5; B-2-6; B-2-10; B-3-3; B-3-4; B-3-5; B-3-6; B-4-3; B-4-4; B-4-5; B-4-6; B-4-10; B-4-11	2.69E+04
Kd_{sw} (L/Kg)	Kd_{sw} value was calculated by using the correlation equation with K_{oc} that is cited in U.S. EPA (1993d) for an assumed organic carbon fraction of 0.075 in suspended sediment. Measured organic carbon in suspended sediment, specific to site conditions, should be used to calculate Kd_{sw}, because the value varies, depending on the fraction of organic carbon in suspended sediment. Recommended Kd_{sw} value was calculated by using the K_{oc} value that is provided in this table.	B-4-16; B-4-18; B-4-24	2.02E+05

TABLE A-3-157

CHEMICAL-SPECIFIC INPUTS FOR 1,2,3,7,8-PENTACHLORODIBENZO(P)DIOXIN (40321-76-4)

Parameter	Reference and Explanation	Equations	Value
Chemical/Physical Properties (Continued)			
Kd_{bs} (cm^3/g)	Kd_{bs} value was calculated by using the correlation equation with K_{oc} that is cited in U.S. EPA (1993d) for an assumed organic carbon fraction of 0.04 in bottom sediment. Measured organic carbon in bottom sediment, specific to site conditions, should be used to calculate Kd_{bs}, because the value varies depending on the fraction of organic carbon in bottom sediment. Recommended Kd_{bs} value was calculated by using the K_{oc} value that is provided in this table.	B-4-16; B-4-25	1.08E+05
ksg $(year)^{-1}$	*Ksg* value was assumed to be 0 due to a lack of data.	B-1-1; B-1-2; B-2-1; B-2-2; B-3-1; B-3-2; B-4-1; B-4-2	0.0
Fv (unitless)	*Fv* value was calculated by using equations cited in Junge (1977) and Bidleman (1988). Recommended value of Fv was calculated by using T_m and *Vp* values that are provided in this table. *Vp* value for this compound was converted to a liquid-phase value before being used in the calculations.	B-1-1; B-2-1; B-2-7; B-2-8; B-3-1; B-3-7; B-3-8; B-4-1; B-4-8; B-4-9; B-4-12; B-5-1	2.19E-01
Biotransfer Factors for Plants			
RCF $(\frac{\mu g/g\ DW\ plant}{\mu g/mL\ soil\ water})$	*RCF* value was calculated by using the correlation equation with K_{ow} that is cited in Briggs (1982). Recommended value was calculated by using the K_{ow} value that is provided in this table. The value was then converted to a dry weight basis by using a moisture content of 87 percent.	B-2-10	3.01E+04
$Br_{rootveg}$ $(\frac{\mu g/g\ DW\ plant}{\mu g/g\ soil})$	$Br_{rootveg}$ value was calculated by dividing the *RCF* value with the Kd_s value provided in this table.	B-2-10	1.12E+00
Br_{ag} $(\frac{\mu g/g\ DW\ plant}{\mu g/g\ soil})$	Br_{ag} value was calculated by using the correlation equation with K_{ow} that is cited in Travis and Arms (1988). No distinction was made between values for aboveground produce and forage. Recommended value was calculated by using the K_{ow} value that is provided in this table.	B-2-9	5.62E-03
Br_{forage} $(\frac{\mu g/g\ DW\ plant}{\mu g/g\ soil})$	Br_{forage} value was calculated by using the correlation equation with K_{ow} that is cited in Travis and Arms (1988). No distinction was made between values for aboveground produce and forage. Recommended value was calculated by using the K_{ow} value that is provided in this table.	B-3-9	5.62E-03
Bv_{ag} $(\frac{\mu g/g\ DW\ plant}{\mu g/g\ air})$	Bv_{ag} value was obtained from Lorber (1995). No distinction was made between aboveground produce and forage.	B-2-8	1.20E+05

TABLE A-3-157

CHEMICAL-SPECIFIC INPUTS FOR 1,2,3,7,8-PENTACHLORODIBENZO(P)DIOXIN (40321-76-4)

Parameter	Reference and Explanation	Equations	Value
Biotransfer Factors for Plants (Continued)			
Bv_{forage} ($\frac{\mu g/g\ DW\ plant}{\mu g/g\ air}$)	Bv_{forage} value was obtained from Lorber (1995). No distinction was made between aboveground produce and forage.	B-3-8	1.20E+05
Biotransfer Factors for Animals			
Ba_{milk} (day/kg FW)	U.S. EPA (1995a)	B-3-11	1.00E-02
Ba_{beef} (day/kg FW)	Ba_{beef} value was calculated by increasing Ba_{milk} values by a factor of 5.43, as discussed in Section A3.3.14.	B-3-10	5.43E-02
Ba_{pork} (day/kg FW)	Ba_{pork} value was calculated by increasing Ba_{milk} values by a factor of 6.57, as discussed in Section A3.3.15.	B-3-12	6.57E-02
Ba_{egg} (L/kg FW tissue)	Ba_{egg} value was calculated by multiplying the BCF value for chicken eggs by a chicken soil consumption rate of 0.02 kg (DW)/day (See Appendix A-3). BCF value for eggs was obtained from Stephens, Petreas, and Hayward (1995) for the high exposure chicken group.	B-3-13	4.71E-02
$Ba_{chicken}$ (L/kg FW tissue)	$Ba_{chicken}$ value was calculated by multiplying the BCF value for chicken by a chicken soil consumption rate of 0.02 kg (DW)/day (See Appendix A-3). BCF value for chicken was obtained from Stephens, Petreas, and Hayward (1995) for the high exposure chicken group.	B-3-14	5.50E-02
BCF_{fish} (L/kg FW tissue)	--	B-4-26	NA
BAF_{fish} (L/kg FW)	--	B-4-27	NA
$BSAF_{fish}$ (unitless, lipid based)	U.S. EPA (1994a)	B-4-28	9.00E-02
Other Parameters			
TEF (unitless)	U.S. EPA (1994a)	--	0.50
Health Benchmarks			
Oral CSF $(mg/kg/day)^{-1}$	--	C-1-8	ND
Inhalation CSF $(mg/kg/day)^{-1}$	--	C-1-7	ND
RfD (mg/kg/day)	--	C-2-3	ND
Inhalation URF $(\mu g/m^3)^{-1}$	--	C-2-1	ND
RfC (mg/m^3)	--	C-2-2	ND

Note:

TABLE A-3-157

CHEMICAL-SPECIFIC INPUTS FOR 1,2,3,7,8-PENTACHLORODIBENZO(P)DIOXIN (40321-76-4)

NA = Not Applicable; ND = No Data Available
All parameters are defined in list of FATE AND TRANSPORT PARAMETERS on page A-3-iii.

TABLE A-3-158

CHEMICAL-SPECIFIC INPUTS FOR 1,2,3,7,8-PENTACHLORODIBENZO(P)FURAN (57117-41-6)

Parameter	Reference and Explanation	Equations	Value
Chemical/Physical Properties			
MW (g/mole)	U.S. EPA (1994a)	--	340.42
T_m (K)	U.S. EPA (1994a)	--	498.1
Vp (atm)	U.S. EPA (1994a)	--	3.58E-12 at 25°C (solid)
S (mg/L)	Homologue group average value obtained from U.S. EPA (1994a).	--	2.40E-04
H (atm·m^3/mol)	U.S. EPA (1994a)	B-1-6; B-2-6; B-2-8; B-3-6; B-4-6; B-4-12; B-4-19	6.20E-06
D_a (cm^2/s)	D_a value was calculated by using Equation A-3-2. Recommended value was calculated by using the *MW* and D_a values that are provided in the tables in Appendix A-3 for 2,3,7,8-TCDF.	B-1-6; B-2-6; B-3-6; B-4-6; B-4-21	1.70E-02
D_w (cm^2/s)	D_w value was calculated using the equation cited in U.S. EPA (1996a).	B-4-20	4.51E-06
K_{ow} (unitless)	U.S. EPA (1992d)	--	6.17E+06
K_{oc} (mL/g)	K_{oc} value was calculated by using the correlation equation with K_{ow} for dioxins and furans that is cited in U.S. EPA (1994a) and U.S. EPA (1994c). Recommended value was calculated by using the recommended K_{ow} value that is provided in this table.	--	3.80E+06
Kd_s (cm^3/g)	Kd_s value was calculated by using the correlation equation with K_{oc} that is cited in U.S. EPA (1993d) for an assumed organic carbon fraction of 0.01 in soil. Measured organic carbon in soil, specific to site conditions, should be used to calculate Kd_s, because the value varies, depending on the fraction of organic carbon in soil. Recommended Kd_s value was calculated by using the K_{oc} value that is provided in this table.	B-1-3; B-1-4; B-1-5; B-1-6; B-2-3; B-2-4; B-2-5; B-2-6; B-2-10; B-3-3; B-3-4; B-3-5; B-3-6; B-4-3; B-4-4; B-4-5; B-4-6; B-4-10; B-4-11	3.80E+04
Kd_{sw} (L/Kg)	Kd_{sw} value was calculated by using the correlation equation with K_{oc} that is cited in U.S. EPA (1993d) for an assumed organic carbon fraction of 0.075 in suspended sediment. Measured organic carbon in suspended sediment, specific to site conditions, should be used to calculate Kd_{sw}, because the value varies, depending on the fraction of organic carbon in suspended sediment. Recommended Kd_{sw} value was calculated by using the K_{oc} value that is provided in this table.	B-4-16; B-4-18; B-4-24	2.85E+05

TABLE A-3-158

CHEMICAL-SPECIFIC INPUTS FOR 1,2,3,7,8-PENTACHLORODIBENZO(P)FURAN (57117-41-6)

Parameter	Reference and Explanation	Equations	Value
Chemical/Physical Properties			
Kd_{bs} (cm^3/g)	Kd_{bs} value was calculated by using the correlation equation with K_{oc} that is cited in U.S. EPA (1993d) for an assumed organic carbon fraction of 0.04 in bottom sediment. Measured organic carbon in bottom sediment, specific to site conditions, should be used to calculate Kd_{bs}, because the value varies depending on the fraction of organic carbon in bottom sediment. Recommended Kd_{bs} value was calculated by using the K_{oc} value that is provided in this table.	B-4-16; B-4-25	1.52E+05
ksg $(year)^{-1}$	*ksg* value assumed to be the same as the *ksg* value calculated for 2,3,4,7,8-PentaCDF. *ksg* value was calculated by using the chemical half-life in soil, as cited in Mackay, Shiu, and Ma (1992).	B-1-1; B-1-2; B-2-1; B-2-2; B-3-1; B-3-2; B-4-1; B-4-2	3.57E-01
Fv (unitless)	*Fv* value was calculated by using equations cited in Junge (1977) and Bidleman (1988). Recommended value of Fv was calculated by using T_m and *Vp* values that are provided in this table. *Vp* value for this compound was converted to a liquid phase value before being used in the calculations.	B-1-1; B-2-1; B-2-7; B-2-8; B-3-1; B-3-7; B-3-8; B-4-1; B-4-8; B-4-9; B-4-12; B-5-1	3.64E-01
Biotransfer Factors for Plants			
RCF $(\frac{\mu g/g\ DW\ plant}{\mu g/mL\ soil\ water})$	*RCF* value was calculated by using the correlation equation with K_{ow} that is cited in Briggs (1982). Recommended value was calculated by using the K_{ow} value that is provided in this table. The value was then converted to a dry weight basis by using a moisture content of 87 percent.	B-2-10	3.93E+04
$Br_{rootveg}$ $(\frac{\mu g/g\ DW\ plant}{\mu g/g\ soil})$	$Br_{rootveg}$ value was calculated by dividing the *RCF* value with the Kd_s value provided in this table.	B-2-10	1.03E+00
Br_{ag} $(\frac{\mu g/g\ DW\ plant}{\mu g/g\ soil})$	Br_{ag} value was calculated by using the correlation equation with K_{ow} that is cited in Travis and Arms (1988). No distinction was made between values for aboveground produce and forage. Recommended value was calculated by using the K_{ow} value that is provided in this table.	B-2-9	4.61E-03
Br_{forage} $(\frac{\mu g/g\ DW\ plant}{\mu g/g\ soil})$	Br_{forage} value was calculated by using the correlation equation with K_{ow} that is cited in Travis and Arms (1988). No distinction was made between values for aboveground produce and forage. Recommended value was calculated by using the K_{ow} value that is provided in this table.	B-3-9	4.61E-03
Bv_{ag} $(\frac{\mu g/g\ DW\ plant}{\mu g/g\ air})$	Bv_{ag} value was obtained from Lorber (1995). No distinction was made between aboveground produce and forage.	B-2-8	4.60E+04

TABLE A-3-158

CHEMICAL-SPECIFIC INPUTS FOR 1,2,3,7,8-PENTACHLORODIBENZO(P)FURAN (57117-41-6)

Parameter	Reference and Explanation	Equations	Value
Biotransfer Factors for Plants (Continued)			
Bv_{forage} ($\frac{\mu g/g\ DW\ plant}{\mu g/g\ air}$)	Bv_{forage} value was obtained from Lorber (1995). No distinction was made between aboveground produce and forage.	B-3-8	4.60E+04
Biotransfer Factors for Animals			
Ba_{milk} (day/kg FW)	U.S. EPA (1995a)	B-3-11	2.00E-03
Ba_{beef} (day/kg FW)	Ba_{beef} value was calculated by increasing Ba_{milk} values by a factor of 5.43, as discussed in Section A3.3.14.	B-3-10	1.09E-02
Ba_{pork} (day/kg FW)	Ba_{pork} value was calculated by increasing Ba_{milk} values by a factor of 6.57, as discussed in Section A3.3.15.	B-3-12	1.31E-02
Ba_{egg} (L/kg FW tissue)	Ba_{egg} value was calculated by multiplying the BCF value for chicken eggs by a chicken soil consumption rate of 0.02 kg (DW)/day (See Appendix A-3). BCF value for eggs was obtained from Stephens, Petreas, and Hayward (1995) for the high exposure chicken group.	B-3-13	ND
$Ba_{chicken}$ (L/kg FW tissue)	$Ba_{chicken}$ value was calculated by multiplying the BCF value for chicken by a chicken soil consumption rate of 0.02 kg (DW)/day (See Appendix A-3). BCF value for chicken was obtained from Stephens, Petreas, and Hayward (1995) for the high exposure chicken group.	B-3-14	ND
BCF_{fish} (L/kg FW tissue)	--	B-4-26	NA
BAF_{fish} (L/kg FW)	--	B-4-27	NA
$BSAF_{fish}$ (unitless, lipid based)	U.S. EPA (1994a)	B-4-28	9.00E-02
Other Parameters			
TEF (unitless)	U.S. EPA (1994a)	--	0.05
Health Benchmarks			
Oral CSF $(mg/kg/day)^{-1}$	--	C-1-8	ND
Inhalation CSF $(mg/kg/day)^{-1}$	--	C-1-7	ND
RfD (mg/kg/day)	--	C-2-3	ND
Inhalation URF $(\mu g/m^3)^{-1}$	--	C-2-1	ND
RfC (mg/m^3)	--	C-2-2	ND

TABLE A-3-158

CHEMICAL-SPECIFIC INPUTS FOR 1,2,3,7,8-PENTACHLORODIBENZO(P)FURAN (57117-41-6)

Note:

NA = Not Applicable; ND = No Data Available

All parameters are defined in list of FATE AND TRANSPORT PARAMETERS on page A-3-iii.

TABLE A-3-159

CHEMICAL-SPECIFIC INPUTS FOR 2,3,4,7,8-PENTACHLORODIBENZO(P)FURAN (57117-31-4)

Parameter	Reference and Explanation	Equations	Value
Chemical/Physical Properties			
MW (g/mole)	U.S. EPA (1994a)	--	340.42
T_m (K)	U.S. EPA (1994a)	--	469.1
Vp (atm)	U.S. EPA (1994a)	--	4.33E-12 at 25°C (solid)
S (mg/L)	U.S. EPA (1994a)	--	2.36E-04
H (atm·m^3/mol)	U.S. EPA (1994a)	B-1-6; B-2-6; B-2-8; B-3-6; B-4-6; B-4-12; B-4-19	6.20E-06
D_a (cm^2/s)	D_a value was calculated by using Equation A-3-2. Recommended value was calculated by using the *MW* and D_a values that are provided in the tables in Appendix A-3 for 2,3,7,8-TCDF.	B-1-6; B-2-6; B-3-6; B-4-6; B-4-21	1.70E-02
D_w (cm^2/s)	D_w value was calculated using the equation cited in U.S. EPA (1996a).	B-4-20	4.51E-06
K_{ow} (unitless)	U.S. EPA (1992d)	--	8.32E+06
K_{oc} (mL/g)	K_{oc} value was calculated by using the correlation equation with K_{ow} for dioxins and furans that is cited in U.S. EPA (1994a) and U.S. EPA (1994c). Recommended value was calculated by using the recommended K_{ow} value that is provided in this table.	--	5.13E+06
Kd_s (cm^3/g)	Kd_s value was calculated by using the correlation equation with K_{oc} that is cited in U.S. EPA (1993d) for an assumed organic carbon fraction of 0.01 in soil. Measured organic carbon in soil, specific to site conditions, should be used to calculate Kd_s, because the value varies, depending on the fraction of organic carbon in soil. Recommended Kd_s value was calculated by using the K_{oc} value that is provided in this table.	B-1-3; B-1-4; B-1-5; B-1-6; B-2-3; B-2-4; B-2-5; B-2-6; B-2-10; B-3-3; B-3-4; B-3-5; B-3-6; B-4-3; B-4-4; B-4-5; B-4-6; B-4-10; B-4-11	5.13E+04
Kd_{sw} (L/Kg)	Kd_{sw} value was calculated by using the correlation equation with K_{oc} that is cited in U.S. EPA (1993d) for an assumed organic carbon fraction of 0.075 in suspended sediment. Measured organic carbon in suspended sediment, specific to site conditions, should be used to calculate Kd_{sw}, because the value varies, depending on the fraction of organic carbon in suspended sediment. Recommended Kd_{sw} value was calculated by using the K_{oc} value that is provided in this table.	B-4-16; B-4-18; B-4-24	3.85E+05

TABLE A-3-159

CHEMICAL-SPECIFIC INPUTS FOR 2,3,4,7,8-PENTACHLORODIBENZO(P)FURAN (57117-31-4)

Parameter	Reference and Explanation	Equations	Value
Chemical/Physical Properties (Continued)			
Kd_{bs} (cm^3/g)	Kd_{bs} value was calculated by using the correlation equation with K_{oc} that is cited in U.S. EPA (1993d) for an assumed organic carbon fraction of 0.04 in bottom sediment. Measured organic carbon in bottom sediment, specific to site conditions, should be used to calculate Kd_{bs}, because the value varies depending on the fraction of organic carbon in bottom sediment. Recommended Kd_{bs} value was calculated by using the K_{oc} value that is provided in this table.	B-4-16; B-4-25	2.05E+05
ksg $(year)^{-1}$	*ksg* value was calculated by using the chemical half-life in soil, as cited in Mackay, Shiu, and Ma (1992).	B-1-1; B-1-2; B-2-1; B-2-2; B-3-1; B-3-2; B-4-1; B-4-2	3.57E-01
Fv (unitless)	*Fv* value was calculated by using equations cited in Junge (1977) and Bidleman (1988). Recommended value of Fv was calculated by using T_m and *Vp* values that are provided in this table. *Vp* value for this compound was converted to a liquid phase value before being used in the calculations.	B-1-1; B-2-1; B-2-7; B-2-8; B-3-1; B-3-7; B-3-8; B-4-1; B-4-8; B-4-9; B-4-12; B-5-1	2.63E-01
Biotransfer Factors for Plants			
RCF $(\frac{\mu g/g\ DW\ plant}{\mu g/mL\ soil\ water})$	*RCF* value was calculated by using the correlation equation with K_{ow} that is cited in Briggs (1982). Recommended value was calculated by using the K_{ow} value that is provided in this table. The value was then converted to a dry weight basis by using a moisture content of 87 percent.	B-2-10	4.95E+04
$Br_{rootveg}$ $(\frac{\mu g/g\ DW\ plant}{\mu g/g\ soil})$	$Br_{rootveg}$ value was calculated by dividing the *RCF* value with the Kd_s value provided in this table.	B-2-10	9.65E-01
Br_{ag} $(\frac{\mu g/g\ DW\ plant}{\mu g/g\ soil})$	Br_{ag} value was calculated by using the correlation equation with K_{ow} that is cited in Travis and Arms (1988). No distinction was made between values for aboveground produce and forage. Recommended value was calculated by using the K_{ow} value that is provided in this table.	B-2-9	3.87E-03
Br_{forage} $(\frac{\mu g/g\ DW\ plant}{\mu g/g\ soil})$	Br_{forage} value was calculated by using the correlation equation with K_{ow} that is cited in Travis and Arms (1988). No distinction was made between values for aboveground produce and forage. Recommended value was calculated by using the K_{ow} value that is provided in this table.	B-3-9	3.87E-03
Bv_{ag} $(\frac{\mu g/g\ DW\ plant}{\mu g/g\ air})$	Bv_{ag} value was obtained from Lorber (1995). No distinction was made between aboveground produce and forage.	B-2-8	4.60E+04

TABLE A-3-159

CHEMICAL-SPECIFIC INPUTS FOR 2,3,4,7,8-PENTACHLORODIBENZO(P)FURAN (57117-31-4)

Parameter	Reference and Explanation	Equations	Value
Biotransfer Factors for Plants (Continued)			
Bv_{forage} $(\frac{\mu g/g\ DW\ plant}{\mu g/g\ air})$	Bv_{forage} value was obtained from Lorber (1995). No distinction was made between aboveground produce and forage.	B-3-8	4.60E+04
Biotransfer Factors for Animals			
Ba_{milk} (day/kg FW)	U.S. EPA (1995a)	B-3-11	9.00E-03
Ba_{beef} (day/kg FW)	Ba_{beef} value was calculated by increasing Ba_{milk} values by a factor of 5.43, as discussed in Section A3.3.14.	B-3-10	4.89E-02
Ba_{pork} (day/kg FW)	Ba_{pork} value was calculated by increasing Ba_{milk} values by a factor of 6.57, as discussed in Section A3.3.15.	B-3-12	5.91E-02
Ba_{egg} (L/kg FW tissue)	Ba_{egg} value was calculated by multiplying the BCF value for chicken eggs by a chicken soil consumption rate of 0.02 kg (DW)/day (See Appendix A-3). BCF value for eggs was obtained from Stephens, Petreas, and Hayward (1995) for the high exposure chicken group.	B-3-13	5.61E-02
$Ba_{chicken}$ (L/kg FW tissue)	$Ba_{chicken}$ value was calculated by multiplying the BCF value for chicken by a chicken soil consumption rate of 0.02 kg (DW)/day (See Appendix A-3). BCF value for chicken was obtained from Stephens, Petreas, and Hayward (1995) for the high exposure chicken group.	B-3-14	7.32E-02
BCF_{fish} (L/kg FW tissue)	--	B-4-26	NA
BAF_{fish} (L/kg FW)	--	B-4-27	NA
$BSAF_{fish}$ (unitless, lipid based)	U.S. EPA (1994a)	B-4-28	9.00E-02
Other Parameters			
TEF (unitless)	U.S. EPA (1994a)	--	0.50
Health Benchmarks			
Oral CSF $(mg/kg/day)^{-1}$	--	C-1-8	ND
Inhalation CSF $(mg/kg/day)^{-1}$	--	C-1-7	ND
RfD (mg/kg/day)	--	C-2-3	ND
Inhalation URF $(\mu g/m^3)^{-1}$	--	C-2-1	ND
RfC (mg/m^3)	--	C-2-2	ND

TABLE A-3-159

CHEMICAL-SPECIFIC INPUTS FOR 2,3,4,7,8-PENTACHLORODIBENZO(P)FURAN (57117-31-4)

Note:

NA = Not Applicable; ND = No Data Available
All parameters are defined in list of FATE AND TRANSPORT PARAMETERS on page A-3-iii.

TABLE A-3-160

CHEMICAL-SPECIFIC INPUTS FOR PENTACHLOROBENZENE (608-93-5)

Parameter	Reference and Explanation	Equations	Value
Chemical/Physical Properties			
MW (g/mole)	Montgomery and Welkom (1991)	--	250.34
T_m (K)	Montgomery and Welkom (1991)	--	358.1
Vp (atm)	Geometric mean value cited in U.S. EPA (1994f)	--	3.10E-06 at 25°C (solid)
S (mg/L)	Geometric mean value cited in U.S. EPA (1994f)	--	3.20E-02
H (atm·m^3/mol)	*H* value was calculated by using the theoretical equation from Lyman, Reehl, and Rosenblatt (1982), which defines the constant. Recommended value was calculated by using the *MW*, *S*, and *Vp* values that are provided in this table.	B-1-6; B-2-6; B-2-8; B-3-6; B-4-6; B-4-12; B-4-19	2.43E-02
D_a (cm^2/s)	D_a value was obtained from CHEMDAT8 database (U.S. EPA 1994d).	B-1-6; B-2-6; B-3-6; B-4-6; B-4-21	1.86E-02
D_w (cm^2/s)	D_w value was obtained from CHEMDAT8 database (U.S. EPA 1994d).	B-4-20	7.34E-06
K_{ow} (unitless)	Geometric mean value cited in U.S. EPA (1994c)	--	1.22E+05
K_{oc} (mL/g)	Geometric mean of measured values obtained from U.S. EPA (1996b).	--	3.21E+04
Kd_s (cm^3/g)	Kd_s value was calculated by using the correlation equation with K_{oc} that is cited in U.S. EPA (1993d) for an assumed organic carbon fraction of 0.01 in soil. Measured organic carbon in soil, specific to site conditions, should be used to calculate Kd_s, because the value varies, depending on the fraction of organic carbon in soil. Recommended Kd_s value was calculated by using the K_{oc} value that is provided in this table.	B-1-3; B-1-4; B-1-5; B-1-6; B-2-3; B-2-4; B-2-5; B-2-6; B-2-10; B-3-3; B-3-4; B-3-5; B-3-6; B-4-3; B-4-4; B-4-5; B-4-6; B-4-10; B-4-11	3.21E+02
Kd_{sw} (L/Kg)	Kd_{sw} value was calculated by using the correlation equation with K_{oc} that is cited in U.S. EPA (1993d) for an assumed organic carbon fraction of 0.075 in suspended sediment. Measured organic carbon in suspended sediment, specific to site conditions, should be used to calculate Kd_{sw}, because the value varies, depending on the fraction of organic carbon in suspended sediment. Recommended Kd_{sw} value was calculated by using the K_{oc} value that is provided in this table.	B-4-16; B-4-18; B-4-24	2.41E+03
Kd_{bs} (cm^3/g)	Kd_{bs} value was calculated by using the correlation equation with K_{oc} that is cited in U.S. EPA (1993d) for an assumed organic carbon fraction of 0.04 in bottom sediment. Measured organic carbon in bottom sediment, specific to site conditions, should be used to calculate Kd_{bs}, because the value varies, depending on the fraction of organic carbon in bottom sediment. Recommended Kd_{bs} value was calculated by using the K_{oc} value that is provided in this table.	B-4-16; B-4-25	1.29E+03

TABLE A-3-160

CHEMICAL-SPECIFIC INPUTS FOR PENTACHLOROBENZENE (608-93-5)

Parameter	Reference and Explanation	Equations	Value
Chemical/Physical Properties (Continued)			
ksg $(year)^{-1}$	*Ksg* value was calculated by using the chemical half-life in soil, as cited in Howard, Boethling, Jarvis, Meylan, and Michalenko (1991).	B-1-2; B-2-2; B-3-2; B-4-2	7.33E-01
Fv (unitless)	*Fv* value was calculated by using equations cited in Junge (1977) and Bidleman (1988). Recommended value of *Fv* was calculated by using T_m and *Vp* values that are provided in this table. *Vp* value for this compound was converted to a liquid-phase value before being used in the calculations.	B-1-1; B-2-1; B-2-7; B-2-8; B-3-1; B-3-7; B-3-8; B-4-1; B-4-8; B-4-9; B-4-12; B-5-1	1.0
Biotransfer Factors for Plants			
RCF $(\frac{\mu g/g\ DW\ plant}{\mu g/mL\ soil\ water})$	*RCF* value was calculated by using the correlation equation with K_{ow} that is cited in Briggs (1982). Recommended value was calculated by using the K_{ow} value that is provided in this table. The value was then converted to a dry weight basis by using a moisture content of 87 percent.	B-2-10	1.93E+03
$Br_{rootveg}$ $(\frac{\mu g/g\ DW\ plant}{\mu g/g\ soil})$	$Br_{rootveg}$ value was calculated by dividing the *RCF* value with the Kd_s value provided in this table.	B-2-10	5.99E+00
Br_{ag} $(\frac{\mu g/g\ DW\ plant}{\mu g/g\ soil})$	Br_{ag} value was calculated by using the correlation equation with K_{ow} that is cited in Travis and Arms (1988). No distinction was made between values for aboveground produce and forage. Recommended value was calculated by using the K_{ow} value that is provided in this table.	B-2-9	4.44E-02
Br_{forage} $(\frac{\mu g/g\ DW\ plant}{\mu g/g\ soil})$	Br_{forage} value was calculated by using the correlation equation with K_{ow} that is cited in Travis and Arms (1988). No distinction was made between values for aboveground produce and forage. Recommended value was calculated by using the K_{ow} value that is provided in this table.	B-3-9	4.44E-02
Bv_{ag} $(\frac{\mu g/g\ DW\ plant}{\mu g/g\ air})$	Bv_{ag} value was calculated by using the correlation equation with K_{ow} and *H* that is cited in Bacci, Calamari, Gaggi, and Vighi (1990); and Bacci, Cerejeira, Gaggi, Chemello, Calamari, and Vighi (1992); then reducing this value by a factor of 100. No distinction was made between values for aboveground produce and forage. Recommended value was calculated, for a temperature (T) of 25°C, by using the *H* and K_{ow} values that are provided in this table.	B-2-8	6.04E-01
Bv_{forage} $(\frac{\mu g/g\ DW\ plant}{\mu g/g\ air})$	Bv_{forage} value was calculated by using the correlation equation with K_{ow} and *H* that is cited in Bacci, Calamari, Gaggi, and Vighi (1990); and Bacci, Cerejeira, Gaggi, Chemello, Calamari, and Vighi (1992); then reducing this value by a factor of 100. No distinction was made between values for aboveground produce and forage. Recommended value was calculated, for a temperature (T) of 25°C, by using the *H* and K_{ow} values that are provided in this table.	B-3-8	6.04E-01

TABLE A-3-160

CHEMICAL-SPECIFIC INPUTS FOR PENTACHLOROBENZENE (608-93-5)

Parameter	Reference and Explanation	Equations	Value
Biotransfer Factors for Animals			
Ba_{milk} (day/kg FW)	Ba_{milk} value was calculated by using the correlation equation with K_{ow} that is cited in Travis and Arms (1988). Recommended value was calculated by using the K_{ow} value that is provided in this table.	B-3-11	9.72E-04
Ba_{beef} (day/kg FW)	Ba_{beef} value was calculated by using the correlation equation with K_{ow} that is cited in Travis and Arms (1988). Recommended value was calculated by using the K_{ow} value that is provided in this table.	B-3-10	3.07E-03
Ba_{pork} (day/kg FW)	Ba_{pork} value was calculated by using thethe fat content ratio of pork to beef (23/19) and multiplying it with the Ba_{beef} value.	B-3-12	3.72E-03
Ba_{egg} (day/kg FW)	Ba_{egg} value was calculated by using the correlation equation with K_{ow} that is cited in California EPA (1993). Recommended value was calculated by using the K_{ow} value that is provided in this table.	B-3-13	9.72E-01
$Ba_{chicken}$ (day/kg FW)	$Ba_{chicken}$ value was calculated by using the fat content ratio of chicken to beef (15/19) and multiplying it with the Ba_{beef} value.	B-3-14	2.43E-03
BCF_{fish} (L/kg FW tissue)	--	B-4-26	NA
BAF_{fish} (L/kg FW)	*BAFs* were used for compounds with a log K_{ow} value above 4.0, as cited in U.S. EPA (1995b). *BAF* values were predicted values calculated by multiplying a food chain multiplier (*FCM*) with a geometric mean of various laboratory measured *BCF*s obtained from various experimental studies cited in U.S. EPA (1998). *FCM*s were obtained from U.S. EPA (1995bc)—See Appendix A-3.	B-4-27	3.61E+04
$BSAF_{fish}$ (unitless)	--	B-4-28	NA
Health Benchmarks			
RfD (mg/kg/day)	U.S. EPA (1997b)	C-1-8	8.0E-04
Oral CSF $(mg/kg/day)^{-1}$	--	C-1-7	ND
RfC (mg/m^3)	Calculated from *RfD* using an inhalation rate of 20 m^3/day and a human body weight of 70 kg.	C-2-3	2.8E-03
Inhalation URF $(\mu g/m^3)^{-1}$	--	C-2-1	ND
Inhalation CSF $(mg/kg/day)^{-1}$	--	C-2-2	ND

Note:

NA = Not applicable
ND = No data available

All parameters are defined in list of FATE AND TRANSPORT PARAMETERS on page A-3-iii.

TABLE A-3-161

CHEMICAL-SPECIFIC INPUTS FOR PENTACHLORONITROBENZENE (82-68-8)

Parameter	Reference and Explanation	Equations	Value
Chemical/Physical Properties			
MW (g/mole)	Budavari, O'Neil, Smith, and Heckelman (1989)	--	295.36
T_m (K)	Budavari, O'Neil, Smith, and Heckelman (1989)	--	417.1
Vp (atm)	Geometric mean value cited in U.S. EPA (1994f). U.S. EPA (1994c) cites value from Howard (1989-1993)	--	3.1E-06 at 25°C (solid)
S (mg/L)	Geometric mean value cited in U.S. EPA (1994f); U.S. EPA (1994c) cites value from Howard, Boethling, Jarvis, Meylan, and Michalenko (1991).	--	3.20E-02
H (atm·m^3/mol)	*H* value was calculated by using the theoretical equation from Lyman, Reehl, and Rosenblatt, (1982), which defines the constant. Recommended value was calculated by using the *MW*, *S* and *Vp* values that are provided in this table.	B-1-6; B-2-6; B-2-8; B-3-6; B-4-6; B-4-12; B-4-19	2.86E-02
D_a (cm^2/s)	D_a value was obtained from CHEMDAT8 database, U.S. EPA (1994d).	B-1-6; B-2-6; B-3-6; B-4-6; B-4-21	1.87E-02
D_w (cm^2/s)	D_w value was obtained from CHEMDAT8 database, U.S. EPA (1994d).	B-4-20	5.0E-06
K_{ow} (unitless)	Geometric mean value cited in U.S. EPA (1994f).	--	4.37E+04
K_{oc} (mL/g)	K_{oc} value was calculated by using the correlation equation with K_{ow} for all nonionizing organics except phthalates, PAHs, dioxins, and furans, as cited in U.S. EPA (1994c). K_{oc} value was calculated by using the recommended K_{ow} value that is provided in this table.	--	5.89E+03
Kd_s (mL/g)	Kd_s value was calculated by using the correlation equation with K_{oc} that is cited in U.S. EPA (1993d) for an assumed fraction organic carbon of 0.01 in soil. Measured organic carbon in soil, specific to site conditions, should be used to calculate Kd_s, because the value varies, depending on the fraction of organic carbon in soil. Recommended Kd_s value was calculated by using the K_{oc} value that is provided in this table.	B-1-3; B-1-4; B-1-5; B-1-6; B-2-3; B-2-4; B-2-5; B-2-6; B-2-10; B-3-3; B-3-4; B-3-5; B-3-6; B-4-3; B-4-4; B-4-5; B-4-6; B-4-10; B-4-11	5.89E+01
Kd_{sw} (L/Kg)	Kd_{sw} value was calculated by using the correlation equation with K_{oc} that is cited in U.S. EPA (1993d) for an assumed organic carbon fraction of 0.075 in suspended sediment. Measured organic carbon in suspended sediment, specific to site conditions, should be used to calculate Kd_{sw}, because the value varies, depending on the fraction of organic carbon in suspended sediment. Recommended Kd_{sw} value was calculated by using the K_{oc} value that is provided in this table.	B-4-16; B-4-18; B-4-24	4.42E+02

TABLE A-3-161

CHEMICAL-SPECIFIC INPUTS FOR PENTACHLORONITROBENZENE (82-68-8)

Parameter	Reference and Explanation	Equations	Value
Kd_{bs} (mL/g)	Kd_{bs} value was calculated by using the correlation equation with K_{oc} that is cited in U.S. EPA (1993d) for an assumed organic carbon fraction of 0.04 in bottom sediment. Measured organic carbon in bottom sediment, specific to site conditions, should be used to calculate Kd_{bs}, because the value varies, depending on the fraction of organic carbon in bottom sediment. Recommended Kd_{bs} value was calculated by using the K_{oc} value that is provided in this table.	B-4-16; B-4-25	2.36E+02
Chemical/Physical Properties (Continued)			
ksg $(year)^{-1}$	*Ksg* value was calculated by using the chemical half-life in soil, as cited in Howard, Boethling, Jarvis, Meylan, and Michalenko (1991).	B-1-2; B-2-2; B-3-2; B-4-2	3.62E-01
Fv (unitless)	*Fv* value was calculated by using equations cited in Junge (1977) and Bidleman (1988). Recommended value of *Fv* was calculated by using *S*, T_m, and *Vp* values that are provided in this table. *Vp* value for this compound was converted to a liquid-phase value before being used in the calculations.	B-1-1; B-2-1; B-2-7; B-2-8; B-3-1; B-3-7; B-3-8; B-4-1; B-4-8; B-4-9; B-4-12; B-5-1	1.0
Biotransfer Factors for Plants			
RCF $(\frac{\mu g/g\ DW\ plant}{\mu g/mL\ soil\ water})$	*RCF* value was calculated by using the correlation equation with K_{ow} that is cited in Briggs (1982). Recommended value was calculated by using the K_{ow} value that is provided in this table. The value was converted to a dry weight basis by using a moisture content of 87 percent.	B-2-10	8.75E+02
$Br_{root\ veg}$ $(\frac{\mu g/g\ DW\ plant}{\mu g/g\ soil})$	$Br_{root\ veg}$ value was calculated by dividing the *RCF* value with the Kd_s value provided in this table (see section A3.4.2 of Appendix A-3).	B-2-10	1.49E+01
Br_{ag} $(\frac{\mu g/g\ DW\ plant}{\mu g/g\ soil})$	Br_{ag} value was calculated by using the correlation equation with K_{ow} that is cited in Travis and Arms (1988). No distinction was made between values for aboveground produce and forage. Recommended value was calculated by using the K_{ow} value that is provided in this table.	B-2-9	8.06E-02
Br_{forage} $(\frac{\mu g/g\ DW\ plant}{\mu g/g\ soil})$	Br_{forage} value was calculated by using the correlation equation with K_{ow} that is cited in Travis and Arms (1988). No distinction was made between values for aboveground produce and forage. Recommended value was calculated by using the K_{ow} value that is provided in this table.	B-3-9	8.06E-02
Bv_{ag} $(\frac{\mu g/g\ DW\ plant}{\mu g/g\ air})$	Bv_{ag} value was calculated by using the correlation equation with K_{ow} and *H* that is cited in Bacci, Calamari, Gaggi, and Vighi (1990); and Bacci, Cerejeira, Gaggi, Chemello, Calamari, and Vighi (1992); then reducing this value by a factor of 100, as recommended by U.S. EPA (1993d). No distinction was made between values for aboveground produce and forage. Recommended value was calculated, for a temperature (T) of 25°C, by using the *H* and K_{ow} values that are provided in this table.	B-2-8	1.71E-01

TABLE A-3-161

CHEMICAL-SPECIFIC INPUTS FOR PENTACHLORONITROBENZENE (82-68-8)

Parameter	Reference and Explanation	Equations	Value
Bv_{forage} ($\frac{\mu g/g\ DW\ plant}{\mu g/g\ air}$)	Bv_{forage} value was calculated by using the correlation equation with K_{ow} and H that is cited in Bacci, Calamari, Gaggi, and Vighi (1990); and Bacci, Cerejeira, Gaggi, Chemello, Calamari, and Vighi (1992); then reducing this value by a factor of 100, as recommended by U.S. EPA (1993d). No distinction was made between values for aboveground produce and forage. Recommended value was calculated, for a temperature (T) of 25°C, by using the H and K_{ow} values that are provided in this table.	B-3-8	1.71E-01
Biotransfer Factors for Animals			
Ba_{milk} (day/kg FW)	Ba_{milk} value was calculated by using the correlation equation with K_{ow} that is cited in Travis and Arms (1988). Recommended value was calculated by using the K_{ow} value that is provided in this table.	B-3-11	3.47E-04
Ba_{beef} (day/kg FW)	Ba_{beef} value was calculated by using the correlation equation with K_{ow} that is cited in Travis and Arms (1988). Recommended value was calculated by using the K_{ow} value that is provided in this table.	B-3-10	1.10E-03
Ba_{pork} (day/kg FW)	Ba_{pork} value was calculated by using the fat content ratio of pork to beef (23/19) and multiplying it with the Ba_{beef} value (see section A3.4.2 of Appendix A-3).	B-3-12	1.33E-03
Ba_{egg} (day/kg FW)	Ba_{egg} value was calculated by using the correlation equation with K_{ow} that is cited in California EPA (1993). Recommended value was calculated by using the K_{ow} value that is provided in this table.	B-3-13	3.47E-01
$Ba_{chicken}$ (day/kg FW)	$Ba_{chicken}$ value was calculated by using the fat content ratio of chicken to beef (15/19) and multiplying it with the Ba_{beef} value (see section A3.4.3 of Appendix A-3).	B-3-14	8.66E-04
BCF_{fish} (L/kg FW tissue)	--	B-4-26	NA
BAF_{fish} (L/kg FW)	*BAFs* were used for compounds with a log K_{ow} value above 4.0, as cited in U.S. EPA (1995b). *BAF* values were predicted values calculated by multiplying a food chain multiplier (*FCM*) with a geometric mean of various laboratory measured *BCF*s obtained from various experimental studies cited in U.S. EPA (1998). *FCM*s were obtained from U.S. EPA (1995bc)—See Appendix A-3.	B-4-27	4.65E+02
$BSAF_{fish}$ (unitless)	--	B-4-28	NA
Health Benchmarks			
RfD (mg/kg/day)	U.S. EPA (1997c)	C-1-8	3.03E-03
Oral CSF $(mg/kg/day)^{-1}$	U.S. EPA (1997c)	C-1-7	2.6E-01
RfC (mg/m^3)	Calculated from *RfD* using an inhalation rate of 20 m^3/day and a human body weight of 70 kg.	C-2-3	1.1E-02
Inhalation URF $(\mu g/m^3)^{-1}$	Calculated from *Oral CSF* using an inhalation rate of 20 m^3/day and a human body weight of 70 kg.	C-2-1	7.4E-05
Inhalation CSF $(mg/kg/day)^{-1}$	Value based on Oral CSF assuming route-to-route extrapolation.	C-2-2	2.6E-01

TABLE A-3-161

CHEMICAL-SPECIFIC INPUTS FOR PENTACHLORONITROBENZENE (82-68-8)

Note:

NA = Not applicable
ND = No data available

All parameters are defined in list of FATE AND TRANSPORT PARAMETERS on page A-3-iii.

TABLE A-3-162

CHEMICAL-SPECIFIC INPUTS FOR PENTACHLOROPHENOL (87-86-5)

Parameter	Reference and Explanation	Equations	Value
Chemical/Physical Properties			
MW (g/mole)	Budavari, O'Neil, Smith, and Heckelman (1989)	--	266.35
T_m (K)	Budavari, O'Neil, Smith, and Heckelman (1989)	--	463
Vp (atm)	Geometric mean value cited in U.S. EPA (1994c)	--	7.11E-07 at 25°C (solid)
S (mg/L)	Geometric mean value cited in U.S. EPA (1994c)	--	1.34E+01
H (atm·m^3/mol)	*H* value was calculated by using the theoretical equation from Lyman, Reehl, and Rosenblatt (1982), which defines the constant. Recommended value was calculated by using the *MW*, *S* and *Vp* values that are provided in this table.	B-1-6; B-2-6; B-2-8; B-3-6; B-4-6; B-4-12; B-4-19	1.41E-05
D_a (cm^2/s)	D_a value was obtained from CHEMDAT8 database, U.S. EPA (1994d).	B-1-6; B-2-6; B-3-6; B-4-6; B-4-21	1.56E-02
D_w (cm^2/s)	D_w value was obtained from CHEMDAT8 database, U.S. EPA (1994d).	B-4-20	8.01E-06
K_{ow} (unitless)	Geometric mean value cited in U.S. EPA (1994c).	--	1.20E+05
K_{oc} (mL/g)	For all ionizing organics, K_{oc} values were estimated on the basis of pH. Estimated values were obtained from U.S. EPA (1994c).	--	pH / K_{oc}: 1 19,949; 2 19,918; 3 19,604; 4 16,942; 5 7,333; 6 1,417; 7 504.9; 8 408.7; 9 399.1; 10 398.1; 11 398.0; 12 398.0; 13 398.0; 14 398.0
Kd_s (mL/g)	Kd_s value was calculated by using the correlation equation with K_{oc} that is cited in U.S. EPA (1993d) for an assumed fraction organic carbon of 0.01 in soil. Measured organic carbon in soil, specific to site conditions, should be used to calculate Kd_s, because the value varies, depending on the fraction of organic carbon in soil. Recommended Kd_s value was calculated by using the K_{oc} value that is provided in this table.	B-1-3; B-1-4; B-1-5; B-1-6; B-2-3; B-2-4; B-2-5; B-2-6; B-2-10; B-3-3; B-3-4; B-3-5; B-3-6; B-4-3; B-4-4; B-4-5; B-4-6; B-4-10; B-4-11	pH / K_{oc}: 1 199.5; 2 199.2; 3 196.0; 4 169.4; 5 73.33; 6 14.17; 7 5.05; 8 4.09; 9 3.99; 10 3.98; 11 3.98; 12 3.98; 13 3.98; 14 3.98

TABLE A-3-162

CHEMICAL-SPECIFIC INPUTS FOR PENTACHLOROPHENOL (87-86-5)

Parameter	Reference and Explanation	Equations	Value
Kd_{sw} (L/Kg)	Kd_{sw} value was calculated by using the correlation equation with K_{oc} that is cited in U.S. EPA (1993d) for an assumed organic carbon fraction of 0.075 in suspended sediment. Measured organic carbon in suspended sediment, specific to site conditions, should be used to calculate Kd_{sw}, because the value varies, depending on the fraction of organic carbon in suspended sediment. Recommended Kd_{sw} value was calculated by using the K_{oc} value that is provided in this table.	B-4-16; B-4-18; B-4-24	pH / K_{oc} 1 1,496 2 1,494 3 1,470 4 1,271 5 550.0 6 106.2 7 37.87 8 30.66 9 29.93 10 29.86 11 29.85 12 29.85 13 29.85 14 29.85
Kd_{bs} (mL/g)	Kd_{bs} value was calculated by using the correlation equation with K_{oc} that is cited in U.S. EPA (1993d) for an assumed organic carbon fraction of 0.04 in bottom sediment. Measured organic carbon in bottom sediment, specific to site conditions, should be used to calculate Kd_{bs}, because the value varies, depending on the fraction of organic carbon in bottom sediment. Recommended Kd_{bs} value was calculated by using the K_{oc} value that is provided in this table.	B-4-16; B-4-25	pH / K_{oc} 1 798.0 2 796.7 3 784.1 4 677.7 5 293.3 6 56.67 7 20.20 8 16.35 9 15.96 10 15.92 11 15.92 12 15.92 13 15.92 14 15.92
ksg $(year)^{-1}$	*Ksg* value was calculated by using the chemical half-life in soil, as cited in Howard, Boethling, Jarvis, Meylan, and Michalenko (1991).	B-1-2; B-2-2; B-3-2; B-4-2	1.42E+00
Fv (unitless)	*Fv* value was calculated by using equations cited in Junge (1977) and Bidleman (1988). Recommended value of *Fv* was calculated by using *S*, T_m, and *Vp* values that are provided in this table. *Vp* value for this compound was converted to a liquid-phase value before being used in the calculations.	B-1-1; B-2-1; B-2-7; B-2-8; B-3-1; B-3-7; B-3-8; B-4-1; B-4-8; B-4-9; B-4-12; B-5-1	1.0
Biotransfer Factors for Plants			
RCF $(\frac{\mu g/g\ DW\ plant}{\mu g/mL\ soil\ water})$	*RCF* value was calculated by using the correlation equation with K_{ow} that is cited in Briggs (1982). Recommended value was calculated by using the K_{ow} value that is provided in this table. The value was converted to a dry weight basis by using a moisture content of 87 percent.	B-2-10	1.90E+03
$Br_{root\ veg}$ $(\frac{\mu g/g\ DW\ plant}{\mu g/g\ soil})$	$Br_{root\ veg}$ value was calculated by dividing the *RCF* value with the Kd_s value provided in this table.	B-2-10	3.77E+02

TABLE A-3-162

CHEMICAL-SPECIFIC INPUTS FOR PENTACHLOROPHENOL (87-86-5)

Parameter	Reference and Explanation	Equations	Value
Br_{ag} ($\frac{\mu g/g\ DW\ plant}{\mu g/g\ soil}$)	Br_{ag} value was calculated by using the correlation equation with K_{ow} that is cited in Travis and Arms (1988). No distinction was made between values for aboveground produce and forage. Recommended value was calculated by using the K_{ow} value that is provided in this table.	B-2-9	4.48E-02
Br_{forage} ($\frac{\mu g/g\ DW\ plant}{\mu g/g\ soil}$)	Br_{forage} value was calculated by using the correlation equation with K_{ow} that is cited in Travis and Arms (1988). No distinction was made between values for aboveground produce and forage. Recommended value was calculated by using the K_{ow} value that is provided in this table.	B-3-9	4.48E-02
Bv_{ag} ($\frac{\mu g/g\ DW\ plant}{\mu g/g\ air}$)	Bv_{ag} value was calculated by using the correlation equation with K_{ow} and H that is cited in Bacci, Calamari, Gaggi, and Vighi (1990); and Bacci, Cerejeira, Gaggi, Chemello, Calamari, and Vighi (1992); then reducing this value by a factor of 100, as recommended by U.S. EPA (1993d). No distinction was made between values for aboveground produce and forage. Recommended value was calculated, for a temperature(T) of 25°C, by using the H and K_{ow} values that are provided in this table.	B-2-8	1.02E+03
Bv_{forage} ($\frac{\mu g/g\ DW\ plant}{\mu g/g\ air}$)	Bv_{forage} value was calculated by using the correlation equation with K_{ow} and H that is cited in Bacci, Calamari, Gaggi, and Vighi (1990); and Bacci, Cerejeira, Gaggi, Chemello, Calamari, and Vighi (1992); then reducing this value by a factor of 100, as recommended by U.S. EPA (1993d). No distinction was made between values for aboveground produce and forage. Recommended value was calculated, for a temperature (T) of 25°C, by using the H and K_{ow} values that are provided in this table.	B-3-8	1.02E+03
Biotransfer Factors for Animals			
Ba_{milk} (day/kg FW)	Ba_{milk} value was calculated by using the correlation equation with K_{ow} that is cited in Travis and Arms (1988). Recommended value was calculated by using the K_{ow} value that is provided in this table.	B-3-11	9.55E-04
Ba_{beef} (day/kg FW)	Ba_{beef} value was calculated by using the correlation equation with K_{ow} that is cited in Travis and Arms (1988). Recommended value was calculated by using the K_{ow} value that is provided in this table.	B-3-10	3.02E-03
Ba_{pork} (day/kg FW)	Ba_{pork} value was calculated by using thethe fat content ratio of pork to beef (23/19) and multiplying it with the Ba_{beef} value.	B-3-12	3.66E-03
Ba_{eggs} (day/kg FW)	Ba_{eggs} value was calculated by using the correlation equation with K_{ow} that is cited in California EPA (1993). Recommended value was calculated by using the K_{ow} value that is provided in this table.	B-3-13	9.55E-01
$Ba_{chicken}$ (day/kg FW)	$Ba_{chicken}$ value was calculated by using the fat content ratio of chicken to beef (15/19) and multiplying it with the Ba_{beef} value.	B-3-14	2.39E-03
BCF_{fish} (L/kg FW tissue)	--	B-4-26	NA
BAF_{fish} (L/kg FW)	*BAFs* were used for compounds with a log K_{ow} value above 4.0, as cited in U.S. EPA (1995b). *BAF* values were predicted values calculated by multiplying a food chain multiplier (*FCM*) with a geometric mean of various laboratory measured *BCF*s obtained from various experimental studies cited in U.S. EPA (1998). *FCM*s were obtained from U.S. EPA (1995bc)—See Appendix A-3.	B-4-27	3.97E+02
$BSAF_{fish}$ (unitless)	--	B-4-28	NA

TABLE A-3-162

CHEMICAL-SPECIFIC INPUTS FOR PENTACHLOROPHENOL (87-86-5)

Parameter	Reference and Explanation	Equations	Value
Health Benchmarks			

TABLE A-3-162

CHEMICAL-SPECIFIC INPUTS FOR PENTACHLOROPHENOL (87-86-5)

Parameter	Reference and Explanation	Equations	Value
RfD (mg/kg/day)	U.S. EPA (1997c)	C-1-8	3.0E-02
Oral CSF $(mg/kg/day)^{-1}$	U.S. EPA (1997b)	C-1-7	1.2E-01
RfC (mg/m^3)	Calculated from *RfD* using an inhalation rate of 20 m^3/day and a human body weight of 70 kg.	C-2-3	1.1E-01
Inhalation URF $(\mu g/m^3)^{-1}$	Calculated from *Oral CSF* using an inhalation rate of 20 m^3/day and a human body weight of 70 kg.	C-2-1	3.4E-05
Inhalation CSF $(mg/kg/day)^{-1}$	Value based on the Oral CSF assuming route-to-route extrapolation	C-2-2	1.2E-01

Note:

NA = Not applicable
ND = No data available

All parameters are defined in of FATE AND TRANSPORT PARAMETERS on page A-3-iii.

TABLE A-3-163

CHEMICAL-SPECIFIC INPUTS FOR PHENANTHRENE (85-01-8)

Parameter	Reference and Explanation	Equations	Value
Chemical/Physical Properties			
MW (g/mole)	Budavari, O'Neil, Smith, and Heckelman (1989)	--	178.22
T_m (K)	Montgomery and Welkom (1991)	--	371.1
Vp (atm)	Geometric mean value calculated from values cited in Montgomery and Welkom (1991).	--	1.35E-03 at 25°C (solid)
S (mg/L)	*S* value cited in Lucius et al. (1992).	--	1.28E+00
H (atm·m^3/mol)	*H* value was calculated by using the theoretical equation from Lyman, Reehl, and Rosenblatt (1982), which defines the constant. Recommended value was calculated by using the *MW*, *S*, and *Vp* values that are provided in this table.	B-1-6; B-2-6; B-2-8; B-3-6; B-4-6; B-4-12; B-4-19	1.88E-01
D_a (cm^2/s)	D_a value was obtained from CHEMDAT8 database (U.S. EPA 1994d).	B-1-6; B-2-6; B-3-6; B-4-6; B-4-21	3.33E-02
D_w (cm^2/s)	D_w value was obtained from CHEMDAT8 database (U.S. EPA 1994d).	B-4-20	7.47E-06
K_{ow} (unitless)	Arithmetic mean value cited in Karickhoff and Long (1995).	--	3.55E+04
K_{oc} (mL/g)	K_{oc} value was calculated by using the correlation equation with K_{ow} for phthalates and PAHs, / all nonionizing organics except phthalates, PAHs, dioxins, and furans, cited in U.S. EPA (1994c). K_{oc} value was calculated by using the recommended K_{ow} value that is provided in this table.	--	5.01E+04
Kd_s (cm^3/g)	Kd_s value was calculated by using the correlation equation with K_{oc} that is cited in U.S. EPA (1993d) for an assumed organic carbon fraction of 0.01 in soil. Measured organic carbon in soil, specific to site conditions, should be used to calculate Kd_s, because the value varies, depending on the fraction of organic carbon in soil. Recommended Kd_s value was calculated by using the K_{oc} value that is provided in this table.	B-1-3; B-1-4; B-1-5; B-1-6; B-2-3; B-2-4; B-2-5; B-2-6; B-3-3; B-3-4; B-3-5; B-3-6; B-4-3; B-4-4; B-4-5; B-4-6; B-4-10; B-4-11	5.01E+02
Kd_{sw} (L/Kg)	Kd_{sw} value was calculated by using the correlation equation with K_{oc} that is cited in U.S. EPA (1993d) for an assumed organic carbon fraction of 0.075 in suspended sediment. Measured organic carbon in suspended sediment, specific to site conditions, should be used to calculate Kd_{sw}, because the value varies, depending on the fraction of organic carbon in suspended sediment. Recommended Kd_{sw} value was calculated by using the K_{oc} value that is provided in this table.	B-4-16; B-4-18; B-4-24	3.76E+03
Kd_{bs} (cm^3/g)	Kd_{bs} value was calculated by using the correlation equation with K_{oc} that is cited in U.S. EPA (1993d) for an assumed organic carbon fraction of 0.04 in bottom sediment. Measured organic carbon in bottom sediment, specific to site conditions, should be used to calculate Kd_{bs}, because the value varies, depending on the fraction of organic carbon in bottom sediment. Recommended Kd_{bs} value was calculated by using the K_{oc} value that is provided in this table.	B-4-16; B-4-25	2.01E+03

TABLE A-3-163

CHEMICAL-SPECIFIC INPUTS FOR PHENANTHRENE (85-01-8)

Parameter	Reference and Explanation	Equations	Value
Chemical/Physical Properties (Continued)			
ksg $(year)^{-1}$	*Ksg* value was calculated by using the chemical half-life in soil, as cited in Howard, Boethling, Jarvis, Meylan, and Michalenko (1991).	B-1-1; B-1-2; B-2-1; B-2-2; B-3-1; B-3-2; B-4-1; B-4-2	1.26E+00
Fv (unitless)	*Fv* value was calculated by using equations cited in Junge (1977) and Bidleman (1988). Recommended value of *Fv* was calculated by using T_m and *Vp* values that are provided in this table. *Vp* value for this compound was converted to a liquid phase value before being used in the calculations.	B-1-1; B-2-1; B-2-7; B-2-8; B-3-1; B-3-7; B-3-8; B-4-1; B-4-8; B-4-9; B-4-12; B-5-1	1.00
Biotransfer Factors for Plants			
RCF $(\frac{\mu g/g\ DW\ plant}{\mu g/mL\ soil\ water})$	*RCF* value was calculated by using the correlation equation with K_{ow} that is cited in Briggs (1982). Recommended value was calculated by using the K_{ow} value that is provided in this table. The value was then converted to a dry weight basis by using a moisture content of 87 percent.	--	7.47E+02
$Br_{rootveg}$ $(\frac{\mu g/g\ DW\ plant}{\mu g/g\ soil})$	$Br_{rootveg}$ value was calculated by dividing the *RCF* value with the Kd_s value provided in this table.	B-2-10	1.49E+00
Br_{ag} $(\frac{\mu g/g\ DW\ plant}{\mu g/g\ soil})$	Br_{ag} value was calculated by using the correlation equation with K_{ow} that is cited in Travis and Arms (1988). No distinction was made between values for aboveground produce and forage. Recommended value was calculated by using the K_{ow} value that is provided in this table.	B-2-9	9.08E-02
Br_{forage} $(\frac{\mu g/g\ DW\ plant}{\mu g/g\ soil})$	Br_{forage} value was calculated by using the correlation equation with K_{ow} that is cited in Travis and Arms (1988). No distinction was made between values for aboveroud produce and forage. Recommended value was calculated by using the K_{ow} value that is provided in this table.	B-3-9	9.08E-02
Bv_{ag} $(\frac{\mu g/g\ DW\ plant}{\mu g/g\ air})$	Bv_{ag} value was calculated by using the correlation equation with K_{ow} and *H* that is cited in Bacci, Calamari, Gaggi, and Vighi (1990); and Bacci, Cerejeira, Gaggi, Chemello, Calamari, and Vighi (1992); then reducing this value by a factor of 100. No distinction was made between values for aboveground produce and forage. Recommended value was calculated, for a temperature (T) of 25°C, by using the *H* and K_{ow} values that are provided in this table.	B-2-8	2.08E-02
Bv_{forage} $(\frac{\mu g/g\ DW\ plant}{\mu g/g\ air})$	Bv_{forage} value was calculated by using the correlation equation with K_{ow} and *H* that is cited in Bacci, Calamari, Gaggi, and Vighi (1990); and Bacci, Cerejeira, Gaggi, Chemello, Calamari, and Vighi (1992); then reducing this value by a factor of 100. No distinction was made between values for aboveground produce and forage. Recommended value was calculated, for a temperature (T) of 25°C, by using the *H* and K_{ow} values that are provided in this table.	B-3-8	2.08E-02

TABLE A-3-163

CHEMICAL-SPECIFIC INPUTS FOR PHENANTHRENE (85-01-8)

Parameter	Reference and Explanation	Equations	Value
Biotransfer Factors for Animals			
Ba_{milk} (day/kg FW)	Ba_{milk} value was calculated by using the correlation equation with K_{ow} that is cited in Travis and Arms (1988). Recommended value was calculated by using the K_{ow} value that is provided in this table.	B-3-11	2.82E-04
Ba_{beef} (day/kg FW)	Ba_{beef} value was calculated by using the correlation equation with K_{ow} that is cited in Travis and Arms (1988). Recommended value was calculated by using the K_{ow} value that is provided in this table.	B-3-10	8.92E-04
Ba_{pork} (day/kg FW)	Ba_{pork} value was calculated by using the fat content ratio of pork to beef (23/19) and multiplying it with the Ba_{beef} value.	B-3-12	1.08E-03
Ba_{egg} (day/kg FW)	Ba_{egg} value was calculated by using the correlation equation with K_{ow} that is cited in California EPA (1993). Recommended value was calculated by using the K_{ow} value that is provided in this table.	B-3-13	2.82E-01
$Ba_{chicken}$ (day/kg FW)	$Ba_{chicken}$ value was calculated by using the fat content ratio of chicken to beef (15/19) and multiplying it with the Ba_{beef} value.	B-3-14	7.04E-04
BCF_{fish} (L/kg FW tissue)	--	B-4-26	NA
BAF_{fish} (L/kg FW)	Default *BAF* value recommended for use by U.S. EPA (1995b), when literature data were not available.	B-4-27	3.30E+03
$BSAF_{fish}$ (unitless)	--	B-4-28	NA
Health Benchmarks			
RfD (mg/kg/day)	--	C-1-8	ND
Oral CSF $(mg/kg/day)^{-1}$	--	C-1-7	NA
RfC (mg/m^3)	--	C-2-3	ND
Inhalation URF $(\mu g/m^3)^{-1}$	--	C-2-1	NA
Inhalation CSF $(mg/kg/day)^{-1}$	--	C-2-2	NA

Note:

NA = Not applicable
ND = No data available

All parameters are defined in list of FATE AND TRANSPORT PARAMETERS on page A-3-iii.

TABLE A-3-164

CHEMICAL-SPECIFIC INPUTS FOR PHENOL (108-95-2)

Parameter	Reference and Explanation	Equations	Value
Chemical/Physical Properties			
MW (g/mole)	Budavari, O'Neil, Smith, and Heckelman (1989)	--	94.11
T_m (K)	Budavari, O'Neil, Smith, and Heckelman (1989)	--	314.0
Vp (atm)	Geometric mean value cited in U.S. EPA (1994c)	--	5.74E-04 at 25°C (solid)
S (mg/L)	Geometric mean value cited in U.S. EPA (1994c)	--	9.08E+04
H (atm·m^3/mol)	*H* value was calculated by using the theoretical equation from Lyman, Reehl, and Rosenblatt (1982), which defines the constant. Recommended value was calculated by using the *MW*, *S*, and *Vp* values that are provided in this table.	B-1-6; B-2-6; B-2-8; B-3-6; B-4-6; B-4-12; B-4-19	5.95E-07
D_a (cm^2/s)	D_a value was obtained from CHEMDAT8 database (U.S. EPA 1994d).	B-1-6; B-2-6; B-3-6; B-4-6; B-4-21	8.27E-02
D_w (cm^2/s)	D_w value was obtained from CHEMDAT8 database (U.S. EPA 1994d).	B-4-20	1.03E-05
K_{ow} (unitless)	Geometric mean value cited in U.S. EPA (1994c)	--	3.00E+01
K_{oc} (mL/g)	For all ionizing organics, K_{oc} values were estimated on the basis of pH. Estimated values were obtained from U.S. EPA (1994c).	--	pH / K_{oc} 1 22.0 2 22.0 3 22.0 4 22.0 5 22.0 6 22.0 7 22.0 8 21.8 9 20.0 10 11.2 11 2.27 12 0.51 13 0.32 14 0.30
Kd_s (cm^3/g)	Kd_s value was calculated by using the correlation equation with K_{oc} that is cited in U.S. EPA (1993d) for an assumed organic carbon fraction of 0.01 in soil. Measured organic carbon in soil, specific to site conditions, should be used to calculate Kd_s, because the value varies, depending on the fraction of organic carbon in soil. Recommended Kd_s value was calculated by using the K_{oc} value that is provided in this table.	B-1-3; B-1-4; B-1-5; B-1-6; B-2-3; B-2-4; B-2-5; B-2-6; B-2-10; B-3-3; B-3-4; B-3-5; B-3-6; B-4-3; B-4-4; B-4-5; B-4-6; B-4-10; B-4-11	2.20E-01

TABLE A-3-164

CHEMICAL-SPECIFIC INPUTS FOR PHENOL (108-95-2)

Parameter	Reference and Explanation	Equations	Value
Chemical/Physical Properties (Continued)			
Kd_{sw} (L/Kg)	Kd_{sw} value was calculated by using the correlation equation with K_{oc} that is cited in U.S. EPA (1993d) for an assumed organic carbon fraction of 0.075 in suspended sediment. Measured organic carbon in suspended sediment, specific to site conditions, should be used to calculate Kd_{sw}, because the value varies, depending on the fraction of organic carbon in suspended sediment. Recommended Kd_{sw} value was calculated by using the K_{oc} value that is provided in this table.	B-4-16; B-4-18; B-4-24	1.65E+00
Kd_{bs} (cm^3/g)	Kd_{bs} value was calculated by using the correlation equation with K_{oc} that is cited in U.S. EPA (1993d) for an assumed organic carbon fraction of 0.04 in bottom sediment. Measured organic carbon in bottom sediment, specific to site conditions, should be used to calculate Kd_{bs}, because the value varies, depending on the fraction of organic carbon in bottom sediment. Recommended Kd_{bs} value was calculated by using the K_{oc} value that is provided in this table.	B-4-16; B-4-25	8.79E-01
ksg $(year)^{-1}$	*ksg* value was calculated by using the chemical half-life in soil, as cited in Howard, Boethling, Jarvis, Meylan, and Michalenko (1991).	B-1-2; B-2-2; B-3-2; B-4-2	2.53E+01
Fv (unitless)	*Fv* value was calculated by using equations cited in Junge (1977) and Bidleman (1988). Recommended value of *Fv* was calculated by using T_m and *Vp* values that are provided in this table. *Vp* value for this compound was converted to a liquid-phase value before being used in the calculations.	B-1-1; B-2-1; B-2-7; B-2-8; B-3-1; B-3-7; B-3-8; B-4-1; B-4-8; B-4-9; B-4-12; B-5-1	1.0
Biotransfer Factors for Plants			
RCF $(\frac{\mu g/g\ DW\ plant}{\mu g/mL\ soil\ water})$	*RCF* value was calculated by using the correlation equation with K_{ow} that is cited in Briggs (1982). Recommended value was calculated by using the K_{ow} value that is provided in this table. The value was then converted to a dry weight basis by using a moisture content of 87 percent.	B-2-10	9.50E+00
$Br_{root\ veg}$ $(\frac{\mu g/g\ DW\ plant}{\mu g/g\ soil})$	$Br_{root\ veg}$ value was calculated by dividing the *RCF* value with the Kd_s value provided in this table.	B-2-9; B-2-10; B-3-9	4.32E+01
Br_{ag} $(\frac{\mu g/g\ DW\ plant}{\mu g/g\ soil})$	Br_{ag} value was calculated by using the correlation equation with K_{ow} that is cited in Travis and Arms (1988). No distinction was made between values for aboveground produce and forage. Recommended value was calculated by using the K_{ow} value that is provided in this table.	B-2-9	5.42E+00
Br_{forage} $(\frac{\mu g/g\ DW\ plant}{\mu g/g\ soil})$	Br_{forage} value was calculated by using the correlation equation with K_{ow} that is cited in Travis and Arms (1988). No distinction was made between values for abovegroud produce and forage. Recommended value was calculated by using the K_{ow} value that is provided in this table.	B-2-10	5.42E+00

TABLE A-3-164

CHEMICAL-SPECIFIC INPUTS FOR PHENOL (108-95-2)

Parameter	Reference and Explanation	Equations	Value
Bv_{ag} ($\frac{\mu g/g\ DW\ plant}{\mu g/g\ air}$)	Bv_{ag} value was calculated by using the correlation equation with K_{ow} and H that is cited in Bacci, Calamari, Gaggi, and Vighi (1990); and Bacci, Cerejeira, Gaggi, Chemello, Calamari, and Vighi (1992); then reducing this value by a factor of 100. No distinction was made between values for aboveground produce and forage. Recommended value was calculated, for a temperature (T) of 25°C, by using the H and K_{ow} values that are provided in this table.	B-2-9	3.52E+00
Bv_{forage} ($\frac{\mu g/g\ DW\ plant}{\mu g/g\ air}$)	Bv_{forage} value was calculated by using the correlation equation with K_{ow} and H that is cited in Bacci, Calamari, Gaggi, and Vighi (1990); and Bacci, Cerejeira, Gaggi, Chemello, Calamari, and Vighi (1992); then reducing this value by a factor of 100. No distinction was made between values for aboveground produce and forage. Recommended value was calculated, for a temperature (T) of 25°C, by using the H and K_{ow} values that are provided in this table.	B-3-9	3.52E+00
Biotransfer Factors for Animals			
Ba_{milk} (day/kg FW)	Ba_{milk} value was calculated by using the correlation equation with K_{ow} that is cited in Travis and Arms (1988). Recommended value was calculated by using the K_{ow} value that is provided in this table.	B-3-11	2.38E-07
Ba_{beef} (day/kg FW)	Ba_{beef} value was calculated by using the correlation equation with K_{ow} that is cited in Travis and Arms (1988). Recommended value was calculated by using the K_{ow} value that is provided in this table.	B-3-10	7.54E-07
Ba_{pork} (day/kg FW)	Ba_{pork} value was calculated by using the fat content ratio of pork to beef (23/19) and multiplying it with the Ba_{beef} value.	B-3-12	9.12E-07
Ba_{eggs} (day/kg FW)	Ba_{eggs} value was calculated by using the correlation equation with K_{ow} that is cited in California EPA (1993). Recommended value was calculated by using the K_{ow} value that is provided in this table.	B-3-13	2.38E-04
$Ba_{chicken}$ (day/kg FW)	$Ba_{chicken}$ value was calculated by using the fat content ratio of chicken to beef (15/19) and multiplying it with the Ba_{beef} value.	B-3-14	5.95E-07
BCF_{fish} (L/kg FW tissue)	*BCFs* were used for compounds with a log K_{ow} value below 4.0, as cited in U.S. EPA (1995b). BCF_{fish} value calculated using the correlation equation with K_{ow} obtained from Veith, Macek, Petrocelli, and Caroll (1980)—See Appendix A-3.	B-4-26	7.81E+00
BAF_{fish} (L/kg FW)	--	B-4-27	NA
$BSAF_{fish}$ (unitless)	--	B-4-28	NA

TABLE A-3-164

CHEMICAL-SPECIFIC INPUTS FOR PHENOL (108-95-2)

Parameter	Reference and Explanation	Equations	Value
Health Benchmarks			
RfD (mg/kg/day)	U.S. EPA (1997b)	C-1-8	6.0E-01
Oral CSF $(mg/kg/day)^{-1}$	--	C-1-7	ND
RfC (mg/m^3)	Calculated from *RfD* using an inhalation rate of 20 m^3/day and a human body weight of 70 kg.	C-2-3	2.1E+00
Inhalation URF $(\mu g/m^3)^{-1}$	--	C-2-1	ND
Inhalation CSF $(mg/kg/day)^{-1}$	--	C-2-2	ND

Note:

NA= Not applicable
ND= No data available

All parameters are defined in list of FATE AND TRANSPORT PARAMETERS on page A-3-iii.

TABLE A-3-165

CHEMICAL-SPECIFIC INPUTS FOR PHORATE (298-02-2)

Parameter	Reference and Explanation	Equations	Value
Chemical/Physical Properties			
MW (g/mole)	Budavari, O'Neil, Smith, and Heckelman (1989)	--	260.4
T_m (K)	--	--	ND
Vp (atm)	*Vp* value cited in Montgomery and Welkom (1991).	--	1.70E-06 at 25°C (liquid)
S (mg/L)	*S* value cited in U.S. EPA (1995b).	--	3.80E+01
H (atm·m^3/mol)	*H* value was calculated by using the theoretical equation from Lyman, Reehl, and Rosenblatt (1982), which defines the constant. Recommended value was calculated by using the *MW*, *S*, and *Vp* values that are provided in this table.	B-1-6; B-2-6; B-2-8; B-3-6; B-4-6; B-4-12; B-4-19	1.16E-05
D_a (cm^2/s)	D_a value was obtained from CHEMDAT8 database (U.S. EPA 1994d).	B-1-6; B-2-6; B-3-6; B-4-6; B-4-21	2.05E-02
D_w (cm^2/s)	D_w value was obtained from CHEMDAT8 database (U.S. EPA 1994d).	B-4-20	5.88E-06
K_{ow} (unitless)	Arithmetic mean value cited in Karickhoff and Long (1995).	--	6.46E+03
K_{oc} (mL/g)	K_{oc} value was calculated by using the correlation equation with K_{ow} for phthalates and PAHs, / all nonionizing organics except phthalates, PAHs, dioxins, and furans, cited in U.S. EPA (1994c). K_{oc} value was calculated by using the recommended K_{ow} value that is provided in this table.	--	1.33E+03
Kd_s (cm^3/g)	Kd_s value was calculated by using the correlation equation with K_{oc} that is cited in U.S. EPA (1993d) for an assumed organic carbon fraction of 0.01 in soil. Measured organic carbon in soil, specific to site conditions, should be used to calculate Kd_s, because the value varies, depending on the fraction of organic carbon in soil. Recommended Kd_s value was calculated by using the K_{oc} value that is provided in this table.	B-1-3; B-1-4; B-1-5; B-1-6; B-2-3; B-2-4; B-2-5; B-2-6; B-2-10; B-3-3; B-3-4; B-3-5; B-3-6; B-4-3; B-4-4; B-4-5; B-4-6; B-4-10; B-4-11	1.33E+01
Kd_{sw} (L/Kg)	Kd_{sw} value was calculated by using the correlation equation with K_{oc} that is cited in U.S. EPA (1993d) for an assumed organic carbon fraction of 0.075 in suspended sediment. Measured organic carbon in suspended sediment, specific to site conditions, should be used to calculate Kd_{sw}, because the value varies, depending on the fraction of organic carbon in suspended sediment. Recommended Kd_{sw} value was calculated by using the K_{oc} value that is provided in this table.	B-4-16; B-4-18; B-4-24	9.96E+01
Kd_{bs} (cm^3/g)	Kd_{bs} value was calculated by using the correlation equation with K_{oc} that is cited in U.S. EPA (1993d) for an assumed organic carbon fraction of 0.04 in bottom sediment. Measured organic carbon in bottom sediment, specific to site conditions, should be used to calculate Kd_{bs}, because the value varies, depending on the fraction of organic carbon in bottom sediment. Recommended Kd_{bs} value was calculated by using the K_{oc} value that is provided in this table.	B-4-16; B-4-25	5.31E+01

TABLE A-3-165

CHEMICAL-SPECIFIC INPUTS FOR PHORATE (298-02-2)

Parameter	Reference and Explanation	Equations	Value
Chemical/Physical Properties (Continued)			
ksg $(year)^{-1}$	*Ksg value* was assumed to be zero due to a lack of data.	B-1-2; B-2-2; B-3-2; B-4-2	0.0
Fv (unitless)	*Fv* value was calculated by using the equation cited in Junge (1977). Recommended value of *Fv* was calculated by using the *Vp* value that is provided in the table.	B-1-1; B-2-1; B-2-7; B-2-8; B-3-1; B-3-7; B-3-8; B-4-1; B-4-8; B-4-9; B-4-12; B-5-1	1.00
Biotransfer Factors for Plants			
RCF $(\frac{\mu g/g\ DW\ plant}{\mu g/mL\ soil\ water})$	*RCF* value was calculated by using the correlation equation with K_{ow} that is cited in Briggs (1982). Recommended value was calculated by using the K_{ow} value that is provided in this table. The value was then converted to a dry weight basis by using a moisture content of 87 percent.	B-2-10	2.06E+02
$Br_{rootveg}$ $(\frac{\mu g/g\ DW\ plant}{\mu g/g\ soil})$	$Br_{rootveg}$ value was calculated by dividing the *RCF* value with the Kd_s value provided in this table.	B-2-10	1.55E+01
Br_{ag} $(\frac{\mu g/g\ DW\ plant}{\mu g/g\ soil})$	Br_{ag} value was calculated by using the correlation equation with K_{ow} that is cited in Travis and Arms (1988). No distinction was made between values for aboveground produce and forage. Recommended value was calculated by using the K_{ow} value that is provided in this table.	B-2-9	2.43E-01
Br_{forage} $(\frac{\mu g/g\ DW\ plant}{\mu g/g\ soil})$	Br_{forage} value was calculated by using the correlation equation with K_{ow} that is cited in Travis and Arms (1988). No distinction was made between values for abovegroud produce and forage. Recommended value was calculated by using the K_{ow} value that is provided in this table.	B-3-9	2.43E-01
Bv_{ag} $(\frac{\mu g/g\ DW\ plant}{\mu g/g\ air})$	Bv_{ag} value was calculated by using the correlation equation with K_{ow} and *H* that is cited in Bacci, Calamari, Gaggi, and Vighi (1990); and Bacci, Cerejeira, Gaggi, Chemello, Calamari, and Vighi (1992); then reducing this value by a factor of 100. No distinction was made between values for aboveground produce and forage. Recommended value was calculated, for a temperature (T) of 25°C, by using the *H* and K_{ow} values that are provided in this table.	B-2-8	5.48E+01
Bv_{forage} $(\frac{\mu g/g\ DW\ plant}{\mu g/g\ air})$	Bv_{forage} value was calculated by using the correlation equation with K_{ow} and *H* that is cited in Bacci, Calamari, Gaggi, and Vighi (1990); and Bacci, Cerejeira, Gaggi, Chemello, Calamari, and Vighi (1992); then reducing this value by a factor of 100. No distinction was made between values for aboveground produce and forage. Recommended value was calculated, for a temperature (T) of 25°C, by using the *H* and K_{ow} values that are provided in this table.	B-3-8	5.48E+01

TABLE A-3-165

CHEMICAL-SPECIFIC INPUTS FOR PHORATE (298-02-2)

Parameter	Reference and Explanation	Equations	Value
Biotransfer Factors for Animals			
Ba_{milk} (day/kg FW)	Ba_{milk} value was calculated by using the correlation equation with K_{ow} that is cited in Travis and Arms (1988). Recommended value was calculated by using the K_{ow} value that is provided in this table.	B-3-11	5.13E-05
Ba_{beef} (day/kg FW)	Ba_{beef} value was calculated by using the correlation equation with K_{ow} that is cited in Travis and Arms (1988). Recommended value was calculated by using the K_{ow} value that is provided in this table.	B-3-10	1.62E-04
Ba_{pork} (day/kg FW)	Ba_{pork} value was calculated by using the fat content ratio of pork to beef (23/19) and multiplying it with the Ba_{beef} value.	B-3-12	1.96E-04
Ba_{egg} (day/kg FW)	Ba_{egg} value was calculated by using the correlation equation with K_{ow} that is cited in California EPA (1993). Recommended value was calculated by using the K_{ow} value that is provided in this table.	B-3-13	5.13E-02
$Ba_{chicken}$ (day/kg FW)	$Ba_{chicken}$ value was calculated by using the fat content ratio of chicken to beef (15/19) and multiplying it with the Ba_{beef} value.	B-3-14	1.28E-04
BCF_{fish} (L/kg FW tissue)	*BCFs* were used for compounds with a log K_{ow} value below 4.0, as cited in U.S. EPA (1995b). BCF_{fish} value calculated using the correlation equation with K_{ow} obtained from Veith, Macek, Petrocelli, and Caroll (1980)—See Appendix A-3.	B-4-26	4.63E+02
BAF_{fish} (L/kg FW)	--	B-4-27	NA
$BSAF_{fish}$ (unitless)	--	B-4-28	NA
Health Benchmarks			
RfD (mg/kg/day)	U.S.EPA (1997c)	C-1-8	2.0E-04
Oral CSF $(mg/kg/day)^{-1}$	--	C-1-7	ND
RfC (mg/m^3)	Calculated from *RfD* using an inhalation rate of 20 m^3/day and a human body weight of 70 kg.	C-2-3	7.0E-04
Inhalation URF $(\mu g/m^3)^{-1}$	--	C-2-1	ND
Inhalation CSF $(mg/kg/day)^{-1}$	--	C-2-2	ND

Note:

NA = Not applicable
ND = No data available

All parameters are defined in list of FATE AND TRANSPORT PARAMETERS on page A-3-iii.

TABLE A-3-166

CHEMICAL-SPECIFIC INPUTS FOR PHTHALIC ANHYDRIDE (85-44-9)

Parameter	Reference and Explanation	Equations	Value
Chemical/Physical Properties			
MW (g/mole)	Budavari, O'Neil, Smith, and Heckelman (1989)	--	148.11
T_m (K)	Budavari, O'Neil, Smith, and Heckelman (1989)	--	403.9
Vp (atm)	Howard (1989-1993)	--	2.63E-07 at 25°C (solid)
S (mg/L)	Howard (1989-1993)	--	6.20E+03
H (atm·m^3/mol)	*H* value was calculated by using the theoretical equation from Lyman, Reehl, and Rosenblatt (1982), which defines the constant. Recommended value was calculated by using the *MW*, *S*, and *Vp* values that are provided in this table.	B-1-6; B-2-6; B-2-8; B-3-6; B-4-6; B-4-12; B-4-19	6.28E-09
D_a (cm^2/s)	D_a value was obtained from CHEMDAT8 database (U.S. EPA 1994d).	B-1-6; B-2-6; B-3-6; B-4-6; B-4-21	4.04E-02
D_w (cm^2/s)	D_w value was obtained from CHEMDAT8 database (U.S. EPA 1994d).	B-4-20	8.97E-06
K_{ow} (unitless)	NC DEHNR (1997)	--	2.5E-01
K_{oc} (mL/g)	K_{oc} value was calculated by using the correlation equation with K_{ow} for all nonionizing organics except phthalates, PAHs, dioxins, and furans as cited in U.S. EPA (1994c). K_{oc} value was calculated by using the recommended K_{ow} value that is provided in this table.	--	4.80E-01
Kd_s (cm^3/g)	Kd_s value was calculated by using the correlation equation with K_{oc} that is cited in U.S. EPA (1993d) for an assumed fraction organic carbon of 0.01 in soil. Measured organic carbon in soil, specific to site conditions, should be used to calculate Kd_s, because the value varies, depending on the fraction of organic carbon in soil. Recommended Kd_s value was calculated by using the K_{oc} value that is provided in this table.	B-1-3; B-1-4; B-1-5; B-1-6; B-2-3; B-2-4; B-2-5; B-2-6; B-2-10; B-3-3; B-3-4; B-3-5; B-3-6; B-4-3; B-4-4; B-4-5; B-4-6; B-4-10; B-4-11	4.80E-03
Kd_{sw} (L/Kg)	Kd_{sw} value was calculated by using the correlation equation with K_{oc} that is cited in U.S. EPA (1993d) for an assumed organic carbon fraction of 0.075 in suspended sediment. Measured organic carbon in suspended sediment, specific to site conditions, should be used to calculate Kd_{sw}, because the value varies, depending on the fraction of organic carbon in suspended sediment. Recommended Kd_{sw} value was calculated by using the K_{oc} value that is provided in this table.	B-4-16; B-4-18; B-4-24	3.60E-02
Kd_{bs} (cm^3/g)	Kd_{bs} value was calculated by using the correlation equation with K_{oc} that is cited in U.S. EPA (1993d) for an assumed organic carbon of 0.04 in bottom sediment. Measured organic carbon in bottom sediment, specific to site conditions, should be used to calculate Kd_{bs}, because the value varies depending on the fraction of organic fraction in bottom sediment. Recommended Kd_{bs} value was calculated by using the K_{oc} value that is provided in this table.	B-4-16; B-4-25	1.92E-02

TABLE A-3-166

CHEMICAL-SPECIFIC INPUTS FOR PHTHALIC ANHYDRIDE (85-44-9)

Parameter	Reference and Explanation	Equations	Value
Chemical/Physical Properties (Continued)			
ksg (year)$^{-1}$	*Ksg* value was calculated by using the chemical half-life in soil, as cited in Howard, Boethling, Jarvis, Meylan, and Michalenko (1991).	B-1-2; B-2-2; B-3-2; B-4-2	1.35E+04
Fv (unitless)	*Fv* value was calculated by using equations cited in Junge (1977) and Bidleman (1988). Recommended value of *Fv* was calculated by using *S*, T_m, and *Vp* values that are provided in this table. *Vp* value for this compound was converted to a liquid-phase value before being used in the calculations.	B-1-1; B-2-1; B-2-7; B-2-8; B-3-1; B-3-7; B-3-8; B-4-1; B-4-8; B-4-9; B-4-12; B-5-1	1.0
Biotransfer Factors for Plants			
RCF $(\frac{\mu g/g\ DW\ plant}{\mu g/mL\ soil\ water})$	*RCF* value was calculated by using the correlation equation with K_{ow} that is cited in Briggs (1982). Recommended value was calculated by using the K_{ow} value that is provided in this table. The value was converted to a dry weight basis by using a moisture content of 87 percent.	B-2-10	6.39E+00
$Br_{root\ veg}$ $(\frac{\mu g/g\ DW\ plant}{\mu g/g\ soil})$	$Br_{root\ veg}$ value was calculated by dividing the *RCF* value with the Kd_s value provided in this table.	B-2-10	1.33E+03
Br_{ag} $(\frac{\mu g/g\ DW\ plant}{\mu g/g\ soil})$	Br_{ag} value was calculated by using the correlation equation with K_{ow} that is cited in Travis and Arms (1988). No distinction was made between values for aboveground produce and forage. Recommended value was calculated by using the K_{ow} value that is provided in this table.	B-2-9	8.63E+01
Br_{forage} $(\frac{\mu g/g\ DW\ plant}{\mu g/g\ soil})$	Br_{forage} value was calculated by using the correlation equation with K_{ow} that is cited in Travis and Arms (1988). No distinction was made between values for aboveground produce and forage. Recommended value was calculated by using the K_{ow} value that is provided in this table.	B-3-9	8.63E+01
Bv_{ag} $(\frac{\mu g/g\ DW\ plant}{\mu g/g\ air})$	Bv_{ag} value was calculated by using the correlation equation with K_{ow} and *H* that is cited in Bacci, Calamari, Gaggi, and Vighi (1990); and Bacci, Cerejeira, Gaggi, Chemello, Calamari, and Vighi (1992); then reducing this value by a factor of 100, as recommended by U.S. EPA (1993d). No distinction was made between values for aboveground produce and forage. Recommended value was calculated, for a temperature (T) of 25°C, by using the *H* and K_{ow} values that are provided in this table.	B-2-8	2.03E+00
Bv_{forage} $(\frac{\mu g/g\ DW\ plant}{\mu g/g\ air})$	Bv_{forage} value was calculated by using the correlation equation with K_{ow} and *H* that is cited in Bacci, Calamari, Gaggi, and Vighi (1990); and Bacci, Cerejeira, Gaggi, Chemello, Calamari, and Vighi (1992); then reducing this value by a factor of 100, as recommended by U.S. EPA (1993d). No distinction was made between values for aboveground produce and forage. Recommended value was calculated, for a temperature (T) of 25°C, by using the *H* and K_{ow} values that are provided in this table.	B-3-8	2.03E+00

TABLE A-3-166

CHEMICAL-SPECIFIC INPUTS FOR PHTHALIC ANHYDRIDE (85-44-9)

Parameter	Reference and Explanation	Equations	Value
Biotransfer Factors for Animals			
Ba_{milk} (day/kg FW)	Ba_{milk} value was calculated by using the correlation equation with K_{ow} that is cited in Travis and Arms (1988). Recommended value was calculated by using the K_{ow} value that is provided in this table.	B-3-11	1.99E-09
Ba_{beef} (day/kg FW)	Ba_{beef} value was calculated by using the correlation equation with K_{ow} that is cited in Travis and Arms (1988). Recommended value was calculated by using the K_{ow} value that is provided in this table.	B-3-10	6.28E-09
Ba_{pork} (day/kg FW)	Ba_{pork} value was calculated by using the fat content ratio of pork to beef (23/19) and multiplying it with the Ba_{beef} value.	B-3-12	7.60E-09
Ba_{egg} (day/kg FW)	Ba_{egg} value was calculated by using the correlation equation with K_{ow} that is cited in California EPA (1993). Recommended value was calculated by using the K_{ow} value that is provided in this table.	B-3-13	1.99E-06
$Ba_{chicken}$ (day/kg FW)	$Ba_{chicken}$ value was calculated by using the fat content ratio of chicken to beef (15/19) and multiplying it with the Ba_{beef} value.	B-3-14	4.96E-09
BCF_{fish} (L/kg, FW tissue)	*BCFs* were used for compounds with a log K_{ow} value below 4.0, as cited in U.S. EPA (1995b). BCF_{fish} value calculated using the correlation equation with K_{ow} obtained from Veith, Macek, Petrocelli, and Caroll (1980)—See Appendix A-3.	B-4-26	2.05E-01
BAF_{fish} (L/kg FW)	--	B-4-27	NA
$BSAF_{fish}$ (unitless)	--	B-4-28	NA
Health Benchmarks			
RfD (mg/kg/day)	U.S. EPA (1997c)	C-1-8	2.0E+00
Oral CSF $(mg/kg/day)^{-1}$	--	C-1-7	ND
RfC (mg/m^3)	U.S. EPA (1997c)	C-2-3	1.2E-01
Inhalation URF $(\mu g/m^3)^{-1}$	--	C-2-1	ND
Inhalation CSF $(mg/kg/day)^{-1}$	--	C-2-2	ND

Note:

NA = Not applicable
ND = No data available

All parameters are defined in list of FATE AND TRANSPORT PARAMETERS on page A-3-iii.

TABLE A-3-167

CHEMICAL-SPECIFIC INPUTS FOR PRONAMIDE (23950-58-5)

Parameter	Reference and Explanation	Equations	Value
Chemical/Physical Properties			
MW (g/mole)	Budavari, O'Neil, Smith, and Heckelman (1989)	--	256.13
T_m (K)	Budavari, O'Neil, Smith, and Heckelman (1989)	--	428.1
Vp (atm)	*Vp* value cited in U.S. EPA (1995b)	--	5.30E-07 at 25°C (solid)
S (mg/L)	*S* value cited in U.S. EPA (1995b)	--	1.50E+01
H (atm·m^3/mol)	*H* value was calculated by using the theoretical equation from Lyman, Reehl, and Rosenblatt (1982), which defines the constant. Recommended value was calculated by using the *MW*, *S*, and *Vp* values that are provided in this table.	B-1-6; B-2-6; B-2-8; B-3-6; B-4-6; B-4-12; B-4-19	9.05E-06
D_a (cm^2/s)	D_a value was calculated using the equation cited in U.S. EPA (1996a).	B-1-6; B-2-6; B-3-6; B-4-6; B-4-21	4.71E-02
D_w (cm^2/s)	D_w value was calculated using the equation cited in U.S. EPA (1996a).	B-4-20	5.45E-06
K_{ow} (unitless)	Arithmetic mean value cited in Karickhoff and Long (1995)	--	3.24E+03
K_{oc} (mL/g)	K_{oc} value was calculated by using the correlation equation with K_{ow} for all nonionizing organics except phthalates, PAHs, dioxins, and furans, cited in U.S. EPA (1994c). K_{oc} value was calculated by using the recommended K_{ow} value that is provided in this table.	--	7.74E+02
Kd_s (cm^3/g)	Kd_s value was calculated by using the correlation equation with K_{oc} that is cited in U.S. EPA (1993d) for an assumed organic carbon fraction of 0.01 in soil. Measured organic carbon in soil, specific to site conditions, should be used to calculate Kd_s, because the value varies, depending on the fraction of organic carbon in soil. Recommended Kd_s value was calculated by using the K_{oc} value that is provided in this table.	B-1-3; B-1-4; B-1-5; B-1-6; B-2-3; B-2-4; B-2-5; B-2-6; B-2-10; B-3-3; B-3-4; B-3-5; B-3-6; B-4-3; B-4-4; B-4-5; B-4-6; B-4-10; B-4-11	7.74E+00
Kd_{sw} (L/Kg)	Kd_{sw} value was calculated by using the correlation equation with K_{oc} that is cited in U.S. EPA (1993d) for an assumed organic carbon fraction of 0.075 in suspended sediment. Measured organic carbon in suspended sediment, specific to site conditions, should be used to calculate Kd_{sw}, because the value varies, depending on the fraction of organic carbon in suspended sediment. Recommended Kd_{sw} value was calculated by using the K_{oc} value that is provided in this table.	B-4-16; B-4-18; B-4-24	5.81E+01
Kd_{bs} (cm^3/g)	Kd_{bs} value was calculated by using the correlation equation with K_{oc} that is cited in U.S. EPA (1993d) for an assumed organic carbon fraction of 0.04 in bottom sediment. Measured organic carbon in bottom sediment, specific to site conditions, should be used to calculate Kd_{bs}, because the value varies, depending on the fraction of organic carbon in bottom sediment. Recommended Kd_{bs} value was calculated by using the K_{oc} value that is provided in this table.	B-4-16; B-4-25	3.10E+01

TABLE A-3-167

CHEMICAL-SPECIFIC INPUTS FOR PRONAMIDE (23950-58-5)

Parameter	Reference and Explanation	Equations	Value
Chemical/Physical Properties (Continued)			
ksg $(year)^{-1}$	*Ksg* value was assumed to be 0 due to a lack of data.	B-1-2; B-2-2; B-3-2; B-4-2	0.0
Fv (unitless)	*Fv* value was calculated by using equations cited in Junge (1977) and Bidleman (1988). Recommended value of *Fv* was calculated by using T_m and *Vp* values that are provided in this table. *Vp* value for this compound was converted to a liquid-phase value before being used in the calculations.	B-1-1; B-2-1; B-2-7; B-2-8; B-3-1; B-3-7; B-3-8; B-4-1; B-4-8; B-4-9; B-4-12; B-5-1	1.0
Biotransfer Factors for Plants			
RCF $(\frac{\mu g/g\ DW\ plant}{\mu g/mL\ soil\ water})$	*RCF* value was calculated by using the correlation equation with K_{ow} that is cited in Briggs (1982). Recommended value was calculated by using the K_{ow} value that is provided in this table. The value was then converted to a dry weight basis by using a moisture content of 87 percent.	B-2-10	1.23E+02
$Br_{rootveg}$ $(\frac{\mu g/g\ DW\ plant}{\mu g/g\ soil})$	$Br_{rootveg}$ value was calculated by dividing the *RCF* value with the Kd_s value provided in this table.	B-2-10	1.59E+01
Br_{ag} $(\frac{\mu g/g\ DW\ plant}{\mu g/g\ soil})$	Br_{ag} value was calculated by using the correlation equation with K_{ow} that is cited in Travis and Arms (1988). No distinction was made between values for aboveground produce and forage. Recommended value was calculated by using the K_{ow} value that is provided in this table.	B-2-9	3.62E-01
Br_{forage} $(\frac{\mu g/g\ DW\ plant}{\mu g/g\ soil})$	Br_{forage} value was calculated by using the correlation equation with K_{ow} that is cited in Travis and Arms (1988). No distinction was made between values for abovegroud produce and forage. Recommended value was calculated by using the K_{ow} value that is provided in this table.	B-3-9	3.62E-01
Bv_{ag} $(\frac{\mu g/g\ DW\ plant}{\mu g/g\ air})$	Bv_{ag} value was calculated by using the correlation equation with K_{ow} and *H* that is cited in Bacci, Calamari, Gaggi, and Vighi (1990); and Bacci, Cerejeira, Gaggi, Chemello, Calamari, and Vighi (1992); then reducing this value by a factor of 100. No distinction was made between values for aboveground produce and forage. Recommended value was calculated, for a temperature (T) of 25°C, by using the *H* and K_{ow} values that are provided in this table.	B-2-8	3.38E+01
Bv_{forage} $(\frac{\mu g/g\ DW\ plant}{\mu g/g\ air})$	Bv_{forage} value was calculated by using the correlation equation with K_{ow} and *H* that is cited in Bacci, Calamari, Gaggi, and Vighi (1990); and Bacci, Cerejeira, Gaggi, Chemello, Calamari, and Vighi (1992); then reducing this value by a factor of 100. No distinction was made between values for aboveground produce and forage. Recommended value was calculated, for a temperature (T) of 25°C, by using the *H* and K_{ow} values that are provided in this table.	B-3-8	3.38E+01

TABLE A-3-167

CHEMICAL-SPECIFIC INPUTS FOR PRONAMIDE (23950-58-5)

Parameter	Reference and Explanation	Equations	Value
Biotransfer Factors for Animals			
Ba_{milk} (day/kg FW)	Ba_{milk} value was calculated by using the correlation equation with K_{ow} that is cited in Travis and Arms (1988). Recommended value was calculated by using the K_{ow} value that is provided in this table.	B-3-11	2.57E-05
Ba_{beef} (day/kg FW)	Ba_{beef} value was calculated by using the correlation equation with K_{ow} that is cited in Travis and Arms (1988). Recommended value was calculated by using the K_{ow} value that is provided in this table.	B-3-10	8.13E-05
Ba_{pork} (day/kg FW)	Ba_{pork} value was calculated by using thethe fat content ratio of pork to beef (23/19) and multiplying it with the Ba_{beef} value.	B-3-12	9.84E-05
Ba_{egg} (day/kg FW)	Ba_{eggs} value was calculated by using the correlation equation with K_{ow} that is cited in Califrnia EPA (1993). Recommended value was calculated by using the K_{ow} value that is provided in this table.	B-3-13	2.57E-02
$Ba_{chicken}$ (day/kg FW)	$Ba_{chicken}$ value was calculated by using the fat content ratio of chicken to beef (15/19) and multiplying it with the Ba_{beef} value.	B-3-14	6.42E-05
BCF_{fish} (L/kg FW tissue)	*BCFs* were used for compounds with a log K_{ow} value below 4.0, as cited in U.S. EPA (1995b). BCF_{fish} value calculated using the correlation equation with K_{ow} obtained from Veith, Macek, Petrocelli, and Caroll (1980)—See Appendix A-3.	B-4-26	2.74E+02
BAF_{fish} (L/kg FW)	--	B-4-27	NA
$BSAF_{fish}$ (unitless)	--	B-4-28	NA
Health Benchmarks			
RfD (mg/kg/day)	U.S. EPA (1997b)	C-1-8	7.5E-02
Oral CSF $(mg/kg/day)^{-1}$	--	C-1-7	ND
RfC (mg/m^3)	Calculated from *RfD* using an inhalation rate of 20 m^3/day and a human body weight of 70 kg.	C-2-3	2.6E-01
Inhalation URF $(\mu g/m^3)^{-1}$	--	C-2-1	ND
Inhalation CSF $(mg/kg/day)^{-1}$	--	C-2-2	ND

Note:

NA = Not applicable
ND = No data available

All parameters are defined in list of FATE AND TRANSPORT PARAMETERS on page A-3-iii.

TABLE A-3-168

CHEMICAL-SPECIFIC INPUTS FOR PYRENE (129-00-0)

Parameter	Reference and Explanation	Equations	Value
Chemical/Physical Properties			
MW (g/mole)	Budavari, O'Neil, Smith, and Heckelman (1989)	--	202.24
T_m (K)	Montgomery and Welkom (1991)	--	429.1
Vp (atm)	*Vp* value cited in U.S. EPA (1992a).	--	7.36E-12 at 25°C (solid)
S (mg/L)	*S* value cited in U.S. EPA (1992a).	--	1.30E-01
H (atm·m^3/mol)	*H* value was calculated by using the theoretical equation from Lyman, Reehl, and Rosenblatt (1982), which defines the constant. Recommended value was calculated by using the *MW*, *S*, and *Vp* values that are provided in this table.	B-1-6; B-2-6; B-2-8; B-3-6; B-4-6; B-4-12; B-4-19	1.14E-08
D_a (cm^2/s)	D_a value was obtained from CHEMDAT8 database (U.S. EPA 1994d).	B-1-6; B-2-6; B-3-6; B-4-6; B-4-21	2.72E-02
D_w (cm^2/s)	D_w value was obtained from CHEMDAT8 database (U.S. EPA 1994d).	B-4-20	7.14E-06
K_{ow} (unitless)	Geometric mean value cited in U.S. EPA (1994c).	--	1.00E+05
K_{oc} (mL/g)	Geometric mean of measured values obtained from U.S. EPA (1996b).	--	6.80E+04
Kd_s (cm^3/g)	Kd_s value was calculated by using the correlation equation with K_{oc} that is cited in U.S. EPA (1993d) for an assumed organic carbon fraction of 0.01 in soil. Measured organic carbon in soil, specific to site conditions, should be used to calculate Kd_s, because the value varies, depending on the fraction of organic carbon in soil. Recommended Kd_s value was calculated by using the K_{oc} value that is provided in this table.	B-1-3; B-1-4; B-1-5; B-1-6; B-2-3; B-2-4; B-2-5; B-2-6; B-2-10; B-3-3; B-3-4; B-3-5; B-3-6; B-4-3; B-4-4; B-4-5; B-4-6; B-4-10; B-4-11	6.80E+02
Kd_{sw} (L/Kg)	Kd_{sw} value was calculated by using the correlation equation with K_{oc} that is cited in U.S. EPA (1993d) for an assumed organic carbon fraction of 0.075 in suspended sediment. Measured organic carbon in suspended sediment, specific to site conditions, should be used to calculate Kd_{sw}, because the value varies, depending on the fraction of organic carbon in suspended sediment. Recommended Kd_{sw} value was calculated by using the K_{oc} value that is provided in this table.	B-4-16; B-4-18; B-4-24	5.10E+03
Kd_{bs} (cm^3/g)	Kd_{bs} value was calculated by using the correlation equation with K_{oc} that is cited in U.S. EPA (1993d) for an assumed organic carbon fraction of 0.04 in bottom sediment. Measured organic carbon in bottom sediment, specific to site conditions, should be used to calculate Kd_{bs}, because the value varies, depending on the fraction of organic carbon in bottom sediment. Recommended Kd_{bs} value was calculated by using the K_{oc} value that is provided in this table.	B-4-16; B-4-25	2.72E+03

TABLE A-3-168

CHEMICAL-SPECIFIC INPUTS FOR PYRENE (129-00-0)

Parameter	Reference and Explanation	Equations	Value
Chemical/Physical Properties (Continued)			
ksg $(year)^{-1}$	*Ksg* value was calculated by using the chemical half-life in soil, as cited in Mackay, Shiu, and Ma (1992)	B-1-2; B-2-2; B-3-2; B-4-2	1.33E-01
Fv (unitless)	*Fv* value was calculated by using equations cited in Junge (1977) and Bidleman (1988). Recommended value of *Fv* was calculated by using T_m and *Vp* values that are provided in this table. *Vp* value for this compound was converted to a liquid phase value before being used in the calculations.	B-1-1; B-2-1; B-2-7; B-2-8; B-3-1; B-3-7; B-3-8; B-4-1; B-4-8; B-4-9; B-4-12; B-5-1	0.196
Biotransfer Factors for Plants			
RCF $(\frac{\mu g/g\ DW\ plant}{\mu g/mL\ soil\ water})$	*RCF* value was calculated by using the correlation equation with K_{ow} that is cited in Briggs (1982). Recommended value was calculated by using the K_{ow} value that is provided in this table. The value was then converted to a dry weight basis by using a moisture content of 87 percent.	B-2-10	1.66E+03
$Br_{root\ veg}$ $(\frac{\mu g/g\ DW\ plant}{\mu g/g\ soil})$	$Br_{root\ veg}$ value was calculated by dividing the *RCF* value with the Kd_s value provided in this table.	B-2-10	2.44E+00
Br_{ag} $(\frac{\mu g/g\ DW\ plant}{\mu g/g\ soil})$	Br_{ag} value was calculated by using the correlation equation with K_{ow} that is cited in Travis and Arms (1988). No distinction was made between values for aboveground produce and forage. Recommended value was calculated by using the K_{ow} value that is provided in this table.	B-2-9	4.98E-02
Br_{forage} $(\frac{\mu g/g\ DW\ plant}{\mu g/g\ soil})$	Br_{forage} value was calculated by using the correlation equation with K_{ow} that is cited in Travis and Arms (1988). No distinction was made between values for abovegroud produce and forage. Recommended value was calculated by using the K_{ow} value that is provided in this table.	B-3-9	4.98E-02
Bv_{ag} $(\frac{\mu g/g\ DW\ plant}{\mu g/g\ air})$	Bv_{ag} value was calculated by using the correlation equation with K_{ow} and *H* that is cited in Bacci, Calamari, Gaggi, and Vighi (1990); and Bacci, Cerejeira, Gaggi, Chemello, Calamari, and Vighi (1992); then reducing this value by a factor of 100. No distinction was made between values for aboveground produce and forage. Recommended value was calculated, for a temperature (T) of 25°C, by using the *H* and K_{ow} values that are provided in this table.	B-2-8	1.04E+06
Bv_{forage} $(\frac{\mu g/g\ DW\ plant}{\mu g/g\ air})$	Bv_{forage} value was calculated by using the correlation equation with K_{ow} and *H* that is cited in Bacci, Calamari, Gaggi, and Vighi (1990); and Bacci, Cerejeira, Gaggi, Chemello, Calamari, and Vighi (1992); then reducing this value by a factor of 100. No distinction was made between values for aboveground produce and forage. Recommended value was calculated, for a temperature (T) of 25°C, by using the *H* and K_{ow} values that are provided in this table.	B-3-8	1.04E+06

TABLE A-3-168

CHEMICAL-SPECIFIC INPUTS FOR PYRENE (129-00-0)

Parameter	Reference and Explanation	Equations	Value
Biotransfer Factors for Animals			
Ba_{milk} (day/kg FW)	Ba_{milk} value was calculated by using the correlation equation with K_{ow} that is cited in Travis and Arms (1988). Recommended value was calculated by using the K_{ow} value that is provided in this table.	B-3-11	7.98E-04
Ba_{beef} (day/kg FW)	Ba_{beef} value was calculated by using the correlation equation with K_{ow} that is cited in Travis and Arms (1988). Recommended value was calculated by using the K_{ow} value that is provided in this table.	B-3-10	2.52E-03
Ba_{pork} (day/kg FW)	Ba_{pork} value was calculated by using the fat content ratio of pork to beef (23/19) and multiplying it with the Ba_{beef} value.	B-3-12	3.06E-03
Ba_{eggs} (day/kg FW)	Ba_{eggs} value was calculated by using the correlation equation with K_{ow} that is cited in California EPA (1993). Recommended value was calculated by using the K_{ow} value that is provided in this table.	B-3-13	7.98E-01
$Ba_{chicken}$ (day/kg FW)	$Ba_{chicken}$ value was calculated by using the fat content ratio of chicken to beef (15/19) and multiplying it with the Ba_{beef} value.	B-3-14	1.99E-03
BCF_{fish} (L/kg FW tissue)	--	B-4-26	NA
BAF_{fish} (L/kg FW)	*BAFs* were used for compounds with a log K_{ow} value above 4.0, as cited in U.S. EPA (1995b). *BAF* values were predicted values calculated by multiplying a food chain multiplier (*FCM*) with an estimated *BCF*. *BCF*s were estimated using the correlation equation obtained from Veith, Macek, Petrocelli, and Caroll (1980). *FCM*s were obtained from U.S. EPA (1995bc)—See Appendix A-3.	B-4-27	1.19E+04
$BSAF_{fish}$ (unitless)	--	B-4-28	NA
Health Benchmarks			
RfD (mg/kg/day)	U.S.EPA (1997b)	C-1-8	3.0E-02
Oral CSF $(mg/kg/day)^{-1}$	--	C-1-7	ND
RfC (mg/m^3)	Calculated from *RfD* using an inhalation rate of 20 m^3/day and a human body weight of 70 kg.	C-2-3	1.1E-01
Inhalation URF $(\mu g/m^3)^{-1}$	--	C-2-1	ND
Inhalation CSF $(mg/kg/day)^{-1}$	--	C-2-2	ND

Note:

NA = Not applicable
ND = No data available

All parameters are defined in list of FATE AND TRANSPORT PARAMETERS on page A-3-iii.

TABLE A-3-169

CHEMICAL-SPECIFIC INPUTS FOR PYRIDINE (110-86-1)

Parameter	Reference and Explanation	Equations	Value
Chemical/Physical Properties			
MW (g/mole)	Budavari, O'Neil, Smith, and Heckelman (1989)	--	79.10
T_m (K)	Budavari, O'Neil, Smith, and Heckelman (1989)	--	231.5
Vp (atm)	*Vp* value cited in U.S. EPA (1995b)	--	2.60E-02 at 25°C (liquid)
S (mg/L)	*S* value cited in U.S. EPA (1995b)	--	3.00E+02
H (atm·m^3/mol)	*H* value was calculated by using the theoretical equation from Lyman, Reehl, and Rosenblatt (1982), which defines the constant. Recommended value was calculated by using the *MW*, *S*, and *Vp* values that are provided in this table.	B-1-6; B-2-6; B-2-8; B-3-6; B-4-6; B-4-12; B-4-19	6.86E-03
D_a (cm^2/s)	D_a value was obtained from CHEMDAT8 database (U.S. EPA 1994d).	B-1-6; B-2-6; B-3-6; B-4-6; B-4-21	1.10E-01
D_w (cm^2/s)	D_w value was obtained from CHEMDAT8 database (U.S. EPA 1994d).	B-4-20	1.08E-05
K_{ow} (unitless)	Arithmetic mean value cited in Karickhoff and Long (1995)	--	4.68E+00
K_{oc} (mL/g)	K_{oc} value was calculated by using the correlation equation with K_{ow} for all nonionizing organics except phthalates, PAHs, dioxins, and furans, cited in U.S. EPA (1994c). K_{oc} value was calculated by using the recommended K_{ow} value that is provided in this table.	--	4.72E+00
Kd_s (cm^3/g)	Kd_s value was calculated by using the correlation equation with K_{oc} that is cited in U.S. EPA (1993d) for an assumed organic carbon fraction of 0.01 in soil. Measured organic carbon in soil, specific to site conditions, should be used to calculate Kd_s, because the value varies, depending on the fraction of organic carbon in soil. Recommended Kd_s value was calculated by using the K_{oc} value that is provided in this table.	B-1-3; B-1-4; B-1-5; B-1-6; B-2-3; B-2-4; B-2-5; B-2-6; B-2-10; B-3-3; B-3-4; B-3-5; B-3-6; B-4-3; B-4-4; B-4-5; B-4-6; B-4-10; B-4-11	4.72E-02
Kd_{sw} (L/Kg)	Kd_{sw} value was calculated by using the correlation equation with K_{oc} that is cited in U.S. EPA (1993d) for an assumed organic carbon fraction of 0.075 in suspended sediment. Measured organic carbon in suspended sediment, specific to site conditions, should be used to calculate Kd_{sw}, because the value varies, depending on the fraction of organic carbon in suspended sediment. Recommended Kd_{sw} value was calculated by using the K_{oc} value that is provided in this table.	B-4-16; B-4-18; B-4-24	3.54E-01
Kd_{bs} (cm^3/g)	Kd_{bs} value was calculated by using the correlation equation with K_{oc} that is cited in U.S. EPA (1993d) for an assumed organic carbon fraction of 0.04 in bottom sediment. Measured organic carbon in bottom sediment, specific to site conditions, should be used to calculate Kd_{bs}, because the value varies, depending on the fraction of organic carbon in bottom sediment. Recommended Kd_{bs} value was calculated by using the K_{oc} value that is provided in this table.	B-4-16; B-4-25	1.89E-01

TABLE A-3-169

CHEMICAL-SPECIFIC INPUTS FOR PYRIDINE (110-86-1)

Parameter	Reference and Explanation	Equations	Value
Chemical/Physical Properties (Continued)			
ksg $(year)^{-1}$	*ksg* value was calculated by using the chemical half-life in soil, as cited in Howard, Boethling, Jarvis, Meylan, and Michalenko (1991).	B-1-2; B-2-2; B-3-2; B-4-2	3.61E+01
Fv (unitless)	*Fv* value was calculated by using the equation cited in Junge (1977). Recommended value of *Fv* was calculated by using the *Vp* value that is provided in this table.	B-1-1; B-2-1; B-2-7; B-2-8; B-3-1; B-3-7; B-3-8; B-4-1; B-4-8; B-4-9; B-4-12; B-5-1	1.0
Biotransfer Factors for Plants			
RCF $(\frac{\mu g/g\ DW\ plant}{\mu g/mL\ soil\ water})$	*RCF* value was calculated by using the correlation equation with K_{ow} that is cited in Briggs (1982). Recommended value was calculated by using the K_{ow} value that is provided in this table. The value was then converted to a dry weight basis by using a moisture content of 87 percent.	B-2-10	7.07E+00
$Br_{rootveg}$ $(\frac{\mu g/g\ DW\ plant}{\mu g/g\ soil})$	$Br_{rootveg}$ value was calculated by dividing the *RCF* value with the Kd_s value provided in this table.	B-2-10	1.50E+02
Br_{ag} $(\frac{\mu g/g\ DW\ plant}{\mu g/g\ soil})$	Br_{ag} value was calculated by using the correlation equation with K_{ow} that is cited in Travis and Arms (1988). No distinction was made between values for aboveground produce and forage. Recommended value was calculated by using the K_{ow} value that is provided in this table.	B-2-9	1.59E+01
Br_{forage} $(\frac{\mu g/g\ DW\ plant}{\mu g/g\ soil})$	Br_{forage} value was calculated by using the correlation equation with K_{ow} that is cited in Travis and Arms (1988). No distinction was made between values for aboveground produce and forage. Recommended value was calculated by using the K_{ow} value that is provided in this table.	B-3-9	1.59E+01
Bv_{ag} $(\frac{\mu g/g\ DW\ plant}{\mu g/g\ air})$	Bv_{ag} value was calculated by using the correlation equation with K_{ow} and *H* that is cited in Bacci, Calamari, Gaggi, and Vighi (1990); and Bacci, Cerejeira, Gaggi, Chemello, Calamari, and Vighi (1992); then reducing this value by a factor of 100. No distinction was made between values for aboveground produce and forage. Recommended value was calculated, for a temperature (T) of 25°C, by using the *H* and K_{ow} values that are provided in this table.	B-2-8	4.22E-05
Bv_{forage} $(\frac{\mu g/g\ DW\ plant}{\mu g/g\ air})$	Bv_{forage} value was calculated by using the correlation equation with K_{ow} and *H* that is cited in Bacci, Calamari, Gaggi, and Vighi (1990); and Bacci, Cerejeira, Gaggi, Chemello, Calamari, and Vighi (1992); then reducing this value by a factor of 100. No distinction was made between values for aboveground produce and forage. Recommended value was calculated, for a temperature (T) of 25°C, by using the *H* and K_{ow} values that are provided in this table.	B-3-8	4.22E-05

TABLE A-3-169

CHEMICAL-SPECIFIC INPUTS FOR PYRIDINE (110-86-1)

Parameter	Reference and Explanation	Equations	Value
Biotransfer Factors for Animals			
Ba_{milk} (day/kg FW)	Ba_{milk} value was calculated by using the correlation equation with K_{ow} that is cited in Travis and Arms (1988). Recommended value was calculated by using the K_{ow} value that is provided in this table.	B-3-11	3.72E-08
Ba_{beef} (day/kg FW)	Ba_{beef} value was calculated by using the correlation equation with K_{ow} that is cited in Travis and Arms (1988). Recommended value was calculated by using the K_{ow} value that is provided in this table.	B-3-10	1.18E-07
Ba_{pork} (day/kg FW)	Ba_{pork} value was calculated by using the fat content ratio of pork to beef (23/19) and multiplying it with the Ba_{beef} value.	B-3-12	1.42E-07
Ba_{egg} (day/kg FW)	Ba_{egg} value was calculated by using the correlation equation with K_{ow} that is cited in California EPA (1993). Recommended value was calculated by using the K_{ow} value that is provided in this table.	B-3-13	3.72E-05
$Ba_{chicken}$ (day/kg FW)	$Ba_{chicken}$ value was calculated by using the fat content ratio of chicken to beef (15/19) and multiplying it with the Ba_{beef} value.	B-3-14	9.28E-08
BCF_{fish} (L/kg FW tissue)	*BCFs* were used for compounds with a log K_{ow} value below 4.0, as cited in U.S. EPA (1995b). BCF_{fish} value calculated using the correlation equation with K_{ow} obtained from Veith, Macek, Petrocelli, and Caroll (1980)—See Appendix A-3.	B-4-26	1.90E+00
BAF_{fish} (L/kg FW)	--	B-4-27	NA
$BSAF_{fish}$ (unitless)	--	B-4-28	NA
Health Benchmarks			
RfD (mg/kg/day)	U.S. EPA (1997b)	C-1-8	1.0E-03
Oral CSF $(mg/kg/day)^{-1}$	--	C-1-7	ND
RfC (mg/m^3)	Calculated from *RfD* using an inhalation rate of 20 m^3/day and a human body weight of 70 kg.	C-2-3	3.50E-03
Inhalation URF $(\mu g/m^3)^{-1}$	--	C-2-1	ND
Inhalation CSF $(mg/kg/day)^{-1}$	--	C-2-2	ND

Note:

NA= Not applicable
ND= No data available

All parameters are defined in list of FATE AND TRANSPORT PARAMETERS on page A-3-iii.

TABLE A-3-170

CHEMICAL-SPECIFIC INPUTS FOR RONNEL (299-84-3)

Parameter	Reference and Explanation	Equations	Value
Chemical/Physical Properties			
MW (g/mole)	Budavari, O'Neil, Smith, and Heckelman (1989)	--	321.57
T_m (K)	Montgomery and Welkom (1991)	--	314.1
Vp (atm)	--	--	ND
S (mg/L)	--	--	ND
H (atm·m^3/mol)	--	B-1-6; B-2-6; B-2-8; B-3-6; B-4-6; B-4-12; B-4-19	ND
D_a (cm^2/s)	D_a value was calculated using the equation cited in U.S. EPA (1996a).	B-1-6; B-2-6; B-3-6; B-4-6; B-4-21	4.05E-02
D_w (cm^2/s)	D_w value was calculated using the equation cited in U.S. EPA (1996a).	B-4-20	4.69E-06
K_{ow} (unitless)	Recommended K_{ow} value cited in Karickhoff and Long (1995).	--	1.17E+05
K_{oc} (mL/g)	K_{oc} value was calculated by using the correlation equation with K_{ow} for phthalates and PAHs, / all nonionizing organics except phthalates, PAHs, dioxins, and furans, cited in U.S. EPA (1994c). K_{oc} value was calculated by using the recommended K_{ow} value that is provided in this table.	--	1.28E+04
Kd_s (cm^3/g)	Kd_s value was calculated by using the correlation equation with K_{oc} that is cited in U.S. EPA (1993d) for an assumed organic carbon fraction of 0.01 in soil. Measured organic carbon in soil, specific to site conditions, should be used to calculate Kd_s, because the value varies, depending on the fraction of organic carbon in soil. Recommended Kd_s value was calculated by using the K_{oc} value that is provided in this table.	B-1-3; B-1-4; B-1-5; B-1-6; B-2-3; B-2-4; B-2-5; B-2-6; B-2-10; B-3-3; B-3-4; B-3-5; B-3-6; B-4-3; B-4-4; B-4-5; B-4-6; B-4-10; B-4-11	1.28E+02
Kd_{sw} (L/Kg)	Kd_{sw} value was calculated by using the correlation equation with K_{oc} that is cited in U.S. EPA (1993d) for an assumed organic carbon fraction of 0.075 in suspended sediment. Measured organic carbon in suspended sediment, specific to site conditions, should be used to calculate Kd_{sw}, because the value varies, depending on the fraction of organic carbon in suspended sediment. Recommended Kd_{sw} value was calculated by using the K_{oc} value that is provided in this table.	B-4-16; B-4-18; B-4-24	9.56E+02

TABLE A-3-170

CHEMICAL-SPECIFIC INPUTS FOR RONNEL (299-84-3)

Parameter	Reference and Explanation	Equations	Value
Kd_{bs} (cm^3/g)	Kd_{bs} value was calculated by using the correlation equation with K_{oc} that is cited in U.S. EPA (1993d) for an assumed organic carbon fraction of 0.04 in bottom sediment. Measured organic carbon in bottom sediment, specific to site conditions, should be used to calculate Kd_{bs}, because the value varies, depending on the fraction of organic carbon in bottom sediment. Recommended Kd_{bs} value was calculated by using the K_{oc} value that is provided in this table.	B-4-16; B-4-25	5.10E+03
ksg $(year)^{-1}$	*Ksg* value was assumed to be 0 due to a lack of data.	B-1-2; B-2-2; B-3-2; B-4-2	0.0
Fv (unitless)	*Fv* value was assumed to be 1.0 due to a lack of data.	B-1-1; B-2-1; B-2-7; B-2-8; B-3-1; B-3-7; B-3-8; B-4-1; B-4-8; B-4-9; B-4-12; B-5-1	1.0
Biotransfer Factors for Plants			
RCF $(\frac{\mu g/g\ DW\ plant}{\mu g/mL\ soil\ water})$	*RCF* value was calculated by using the correlation equation with K_{ow} that is cited in Briggs (1982). Recommended value was calculated by using the K_{ow} value that is provided in this table. The value was then ocnverted to a dry weight basis by using a moisture content of 87 percent.	B-2-10	1.87E+03
$Br_{root\ veg}$ $(\frac{\mu g/g\ DW\ plant}{\mu g/g\ soil})$	$Br_{root\ veg}$ value was calculated by dividing the *RCF* value with the Kd_s value provided in this table.	B-2-10	1.46E+01
Br_{ag} $(\frac{\mu g/g\ DW\ plant}{\mu g/g\ soil})$	Br_{ag} value was calculated by using the correlation equation with K_{ow} that is cited in Travis and Arms (1988). No distinction was made between values for aboveground produce and forage. Recommended value was calculated by using the K_{ow} value that is provided in this table.	B-2-9	4.55E-02
Br_{forage} $(\frac{\mu g/g\ DW\ plant}{\mu g/g\ soil})$	Br_{forage} value was calculated by using the correlation equation with K_{ow} that is cited in Travis and Arms (1988). No distinction was made between values for aboveground produce and forage. Recommended value was calculated by using the K_{ow} value that is provided in this table.	B-3-9	4.55E-02
$Bv_{leafy\ veg}$ $(\frac{\mu g/g\ DW\ plant}{\mu g/g\ air})$		B-2-8	ND
Bv_{forage} $(\frac{\mu g/g\ DW\ plant}{\mu g/g\ air})$		B-3-8	ND

TABLE A-3-170

CHEMICAL-SPECIFIC INPUTS FOR RONNEL (299-84-3)

Parameter	Reference and Explanation	Equations	Value
Biotransfer Factors for Animals			
Ba_{milk} (day/kg FW)	Ba_{milk} value was calculated by using the correlation equation with K_{ow} that is cited in Travis and Arms (1988). Recommended value was calculated by using the K_{ow} value that is provided in this table.	B-3-11	9.33E-04
Ba_{beef} (day/kg FW)	Ba_{beef} value was calculated by using the correlation equation with K_{ow} that is cited in Travis and Arms (1988). Recommended value was calculated by using the K_{ow} value that is provided in this table.	B-3-10	2.95E-03
Ba_{pork} (day/kg FW)	Ba_{pork} value was calculated by using the fat content ratio of pork to beef (23/19) and multiplying it with the Ba_{beef} value.	B-3-12	3.57E-03
Ba_{egg} (day/kg FW)	Ba_{egg} value was calculated by using the correlation equation with K_{ow} that is cited in California EPA (1993). Recommended value was calculated by using the K_{ow} value that is provided in this table.	B-3-13	9.33E-01
$Ba_{chicken}$ (day/kg FW)	$Ba_{chicken}$ value was calculated by using the fat content ratio of chicken to beef (15/19) and multiplying it with the Ba_{beef} value.	B-3-14	2.33E-03
BCF_{fish} (L/kg FW tissue)	--	B-4-26	NA
BAF_{fish} (L/kg FW)	*BAFs* were used for compounds with a log K_{ow} value above 4.0, as cited in U.S. EPA (1995b). *BAF* values were predicted values calculated by multiplying a food chain multiplier (*FCM*) with an estimated *BCF*. *BCF*s were estimated using the correlation equation obtained from Veith, Macek, Petrocelli, and Caroll (1980). *FCM*s were obtained from U.S. EPA (1995bc)—See Appendix A-3.	B-4-27	1.53E+04
$BSAF_{fish}$ (unitless)	--	B-4-28	NA
Health Benchmarks			
RfD (mg/kg/day)	U.S. EPA (1997c)	C-1-8	5.0E-02
Oral CSF $(mg/kg/day)^{-1}$		C-1-7	ND
RfC (mg/m^3)	Calculated from *RfD* using an inhalation rate of 20 m^3/day and a human body weight of 70 kg.	C-2-3	1.8E-01
Inhalation URF $(\mu g/m^3)^{-1}$		C-2-1	ND
Inhalation CSF $(mg/kg/day)^{-1}$		C-2-2	ND

Note:

NA = Not applicable
ND = No data available

All parameters are defined in list of FATE AND TRANSPORT PARAMETERS on page A-3-iii.

TABLE A-3-171

CHEMICAL-SPECIFIC INPUTS FOR SAFROLE (94-59-7)

Parameter	Reference and Explanation	Equations	Value
Chemical/Physical Properties			
MW (g/mole)	Budavari, O'Neill, Smith, and Heckelman (1989)	--	162.18
T_m (K)	Budavari, O'Neill, Smith, and Heckelman (1989)	--	284.1
Vp (atm)	*Vp* value cited in U.S. EPA (1995b).	--	1.10E-04 at 25°C (liquid)
S (mg/L)	*S* value cited in U.S. EPA (1995b).	--	1.50E+03
H (atm·m^3/mol)	*H* value was calculated by using the theoretical equation from Lyman, Reehl, and Rosenblatt (1982), which defines the constant. Recommended value was calculated by using the *MW*, *S*, and *Vp* values that are provided in this table.	B-1-6; B-2-6; B-2-8; B-3-6; B-4-6; B-4-12; B-4-19	1.19E-05
D_a (cm^2/s)	D_a value was obtained from WATER8 model database (U.S. EPA 1995d).	B-1-6; B-2-6; B-3-6; B-4-6; B-4-21	4.06E-02
D_w (cm^2/s)	D_w value was obtained from WATER8 model database (U.S. EPA 1995d).	B-4-20	7.16E-06
K_{ow} (unitless)	Arithmetic mean value cited in Karickhoff and Long (1995).	--	4.57E+02
K_{oc} (mL/g)	K_{oc} value was calculated by using the correlation equation with K_{ow} for all nonionizing organics except phthalates, PAHs, dioxins, and furans as cited in U.S. EPA (1994c). K_{oc} value was calculated by using the recommended K_{ow} value that is provided in this table.	--	1.68E+02
Kd_s (cm^3/g)	Kd_s value was calculated by using the correlation equation with K_{oc} that is cited in U.S. EPA (1993d) for an assumed fraction organic carbon of 0.01 in soil. Measured organic carbon in soil, specific to site conditions, should be used to calculate Kd_s, because the value varies, depending on the fraction of organic carbon in soil. Recommended Kd_s value was calculated by using the K_{oc} value that is provided in this table.	B-1-3; B-1-4; B-1-5; B-1-6; B-2-3; B-2-4; B-2-5; B-2-6; B-2-10; B-3-3; B-3-4; B-3-5; B-3-6; B-4-3; B-4-4; B-4-5; B-4-6; B-4-10; B-4-11	1.68E+00
Kd_{sw} (L/Kg)	Kd_{sw} value was calculated by using the correlation equation with K_{oc} that is cited in U.S. EPA (1993d) for an assumed organic carbon fraction of 0.075 in suspended sediment. Measured organic carbon in suspended sediment, specific to site conditions, should be used to calculate Kd_{sw}, because the value varies, depending on the fraction of organic carbon in suspended sediment. Recommended Kd_{sw} value was calculated by using the K_{oc} value that is provided in this table.	B-4-16; B-4-18; B-4-24	1.26E+01
Kd_{bs} (cm^3/g)	Kd_{bs} value was calculated by using the correlation equation with K_{oc} that is cited in U.S. EPA (1993d) for an assumed organic carbon of 0.04 in bottom sediment. Measured organic carbon in bottom sediment, specific to site conditions, should be used to calculate Kd_{bs}, because the value varies depending on the fraction of organic fraction in bottom sediment. Recommended Kd_{bs} value was calculated by using the K_{oc} value that is provided in this table.	B-4-16; B-4-25	6.73E+00

TABLE A-3-171

CHEMICAL-SPECIFIC INPUTS FOR SAFROLE (94-59-7)

Parameter	Reference and Explanation	Equations	Value
Chemical/Physical Properties (Continued)			
ksg $(year)^{-1}$	*ksg* value was calculated by using the chemical half-life in soil, as cited in Howard, Boethling, Jarvis, Meylan, and Michalenko (1991).	B-1-2; B-2-2; B-3-2; B-4-2	9.03E+00
Fv (unitless)	*Fv* value was calculated by using the equation cited in Junge (1977). Recommended value of *Fv* was calculated by using the *Vp* value that is provided in this table.	B-1-1; B-2-1; B-2-7; B-2-8; B-3-1; B-3-7; B-3-8; B-4-1; B-4-8; B-4-9; B-4-12; B-5-1	1.0
Biotransfer Factors for Plants			
RCF $(\frac{\mu g/g\ DW\ plant}{\mu g/mL\ soil\ water})$	*RCF* value was calculated by using the correlation equation with K_{ow} that is cited in Briggs (1982). Recommended value was calculated by using the K_{ow} value that is provided in this table. The value was converted to a dry weight basis by using a moisture content of 87 percent.	B-2-10	3.23E+01
$Br_{root\ veg}$ $(\frac{\mu g/g\ DW\ plant}{\mu g/g\ soil})$	$Br_{root\ veg}$ value was calculated by dividing the *RCF* value with the Kd_s value provided in this table.	B-2-10	1.92E+01
Br_{ag} $(\frac{\mu g/g\ DW\ plant}{\mu g/g\ soil})$	Br_{ag} value was calculated by using the correlation equation with K_{ow} that is cited in Travis and Arms (1988). No distinction was made between values for aboveground produce and forage. Recommended value was calculated by using the K_{ow} value that is provided in this table.	B-2-9	1.12E+00
Br_{forage} $(\frac{\mu g/g\ DW\ plant}{\mu g/g\ soil})$	Br_{forage} value was calculated by using the correlation equation with K_{ow} that is cited in Travis and Arms (1988). No distinction was made between values for aboveground produce and forage. Recommended value was calculated by using the K_{ow} value that is provided in this table.	B-3-9	1.12E+00
Bv_{ag} $(\frac{\mu g/g\ DW\ plant}{\mu g/g\ air})$	Bv_{ag} value was calculated by using the correlation equation with K_{ow} and *H* that is cited in Bacci, Calamari, Gaggi, and Vighi (1990); and Bacci, Cerejeira, Gaggi, Chemello, Calamari, and Vighi (1992); then reducing this value by a factor of 100, as recommended by U.S. EPA (1993d). No distinction was made between values for aboveground produce and forage. Recommended value was calculated, for a temperature (T) of 25°C, by using the *H* and K_{ow} values that are provided in this table.	B-2-8	3.20E+00
Bv_{forage} $(\frac{\mu g/g\ DW\ plant}{\mu g/g\ air})$	Bv_{forage} value was calculated by using the correlation equation with K_{ow} and *H* that is cited in Bacci, Calamari, Gaggi, and Vighi (1990); and Bacci, Cerejeira, Gaggi, Chemello, Calamari, and Vighi (1992); then reducing this value by a factor of 100, as recommended by U.S. EPA (1993d). No distinction was made between values for aboveground produce and forage. Recommended value was calculated, for a temperature (T) of 25°C, by using the *H* and K_{ow} values that are provided in this table.	B-3-8	3.20E+00

TABLE A-3-171

CHEMICAL-SPECIFIC INPUTS FOR SAFROLE (94-59-7)

Parameter	Reference and Explanation	Equations	Value
Biotransfer Factors for Animals			
Ba_{milk} (day/kg FW)	Ba_{milk} value was calculated by using the correlation equation with K_{ow} that is cited in Travis and Arms (1988). Recommended value was calculated by using the K_{ow} value that is provided in this table.	B-3-11	3.63E-06
Ba_{beef} (day/kg FW)	Ba_{beef} value was calculated by using the correlation equation with K_{ow} that is cited in Travis and Arms (1988). Recommended value was calculated by using the K_{ow} value that is provided in this table.	B-3-10	1.15E-05
Ba_{pork} (day/kg FW)	Ba_{pork} value was calculated by using the fat content ratio of pork to beef (23/19) and multiplying it with the Ba_{beef} value.	B-3-12	1.39E-05
Ba_{egg} (day/kg FW)	Ba_{egg} value was calculated by using the correlation equation with K_{ow} that is cited in California EPA (1993). Recommended value was calculated by using the K_{ow} value that is provided in this table.	B-3-13	3.63E-03
$Ba_{chicken}$ (day/kg FW)	$Ba_{chicken}$ value was calculated by using the fat content ratio of chicken to beef (15/19) and multiplying it with the Ba_{beef} value.	B-3-14	9.06E-06
BCF_{fish} (L/kg FW tissue)	*BCFs* were used for compounds with a log K_{ow} value below 4.0, as cited in U.S. EPA (1995b). BCF_{fish} value calculated using the correlation equation with K_{ow} obtained from Veith, Macek, Petrocelli, and Caroll (1980)—See Appendix A-3.	B-4-26	6.19E+01
BAF_{fish} (L/kg FW)	--	B-4-27	NA
$BSAF_{fish}$ (unitless)	--	B-4-28	NA
Health Benchmarks			
RfD (mg/kg/day)	--	C-1-8	ND
Oral CSF $(mg/kg/day)^{-1}$	U.S. EPA (1995b)	C-1-7	1.80E-01
RfC (mg/m^3)	--	C-2-3	ND
Inhalation URF $(\mu g/m^3)^{-1}$	Calculated from *Oral CSF* using an inhalation rate of 20 m^3/day and a human body weight of 70 kg.	C-2-1	5.10E-05
Inhalation CSF $(mg/kg/day)^{-1}$	Value based on Oral CSF assuming route-to-route extrapolation.	C-2-2	1.80E-01

Note:

NA= Not applicable
ND= No data available

All parameters are defined in list of FATE AND TRANSPORT PARAMETERS on page A-3-iii.

TABLE A-3-172

CHEMICAL-SPECIFIC INPUTS FOR SELENIUM (7782-49-2)

Parameter	Reference and Explanation	Equations	Value
Chemical/Physical Properties			
MW (g/mole)	Budavari, O'Neil, Smith, and Heckelman (1989)	--	78.96
T_m (^{o}K)	Budavari, O'Neil, Smith, and Heckelman (1989)	--	490.1
Vp (atm)	All metals, except mercury, are assumed to be nonvolatile at ambient temperatures.	--	0.0
S (mg/L)	All metals, except mercury, are assumed to be insoluble in water.	--	0.0
H (atm·m^3/mol)	*H* value is assumed to be zero, because the *Vp* and *S* values are zero for all metals, except mercury.	B-1-6; B-2-6; B-2-8; B-3-6; B-4-6; B-4-12; B-4-19	0.0
D_a (cm^2/s)	D_a value was calculated using the equation cited in U.S. EPA (1996a).	B-1-6; B-2-6; B-3-6; B-4-6; B-4-21	1.03E-01
D_w (cm^2/s)	D_w value was calculated using the equation cited in U.S. EPA (1996a).	B-4-20	1.20E-05
K_{ow} (unitless)	--	--	NA
K_{oc} (mL/g)		--	NA
Kd_s (mL/g)	Kd_s value was obtained from U.S. EPA (1996a), which provides pH-based values that were estimated by using the MINTEQ2 geochemical speciation model.	B-1-3; B-1-4; B-1-5; B-1-6; B-2-3; B-2-4; B-2-5; B-2-6; B-2-10; B-3-3; B-3-4; B-3-5; B-3-6; B-4-3; B-4-4; B-4-5; B-4-6; B-4-10; B-4-11	18 at pH=4.9; 5.0 at pH=6.8; 2.2 at pH=8.0
Kd_{sw} (L/Kg)	Kd_{sw} value is assumed to be same as the Kd_s value, because organic carbon does not play a major role in sorption for the metals, as cited in U.S. EPA (1994f).	B-4-16; B-4-18; B-4-24	18 at pH=4.9; 5.0 at pH=6.8; 2.2 at pH=8.0
Kd_{bs} (mL/g)	Kd_{bs} value is assumed to be same as the Kd_s value, because organic carbon does not play a major role in sorption for the metals, as cited in U.S. EPA (1994f).	B-4-16; B-4-25	18 at pH=4.9; 5.0 at pH=6.8; 2.2 at pH=8.0
ksg (year)$^{-1}$	--	B-1-2; B-2-2; B-3-2; B-4-2	ND

TABLE A-3-172

CHEMICAL-SPECIFIC INPUTS FOR SELENIUM (7782-49-2)

Parameter	Reference and Explanation	Equations	Value
Chemical/Physical Properties (Continued)			
Fv (unitless)	Because they are nonvolatile, metals are assumed to be 100 percent in particulate phase and zero percent in the vapor phase, as cited in U.S. EPA (1994f).	B-1-1; B-2-1; B-2-7; B-2-8; B-3-1; B-3-7; B-3-8; B-4-1; B-4-8; B-4-9; B-4-12; B-5-1	0.0
Biotransfer Factors for Plants			
RCF $(\frac{\mu g/g\ DW\ plant}{\mu g/mL\ soil\ water})$	--	B-2-10	ND
$Br_{rootveg}$ $(\frac{\mu g/g\ DW\ plant}{\mu g/g\ soil})$	$Br_{rootveg}$ value was calculated by multiplying the uptake slope factor with a conversion factor of 2 x 10^9 g/ha soil. The uptake slope factor and the conversion factor were obtained from U.S. EPA (1992b) for root vegetables.	B-2-10	2.20E-02
Br_{ag} $(\frac{\mu g/g\ DW\ plant}{\mu g/g\ soil})$	Br_{ag} value for fruits was calculated by multiplying the uptake slope factor with a conversion factor of 2 x10^9 g/ha soil. The uptake slope factor and the conversion factor were obtained from U.S. EPA (1993e) for garden fruits. Br_{ag} value for vegetables was calculated by weighting the uptake slope factors for garden fruits (75%) and leafy vegetables (25%) and multiplying the result with a conversion factor of 2 x10^9 g/ha soil. The uptake slope factors and the conversion factor were obtained from U.S. EPA (1993e). The weighted average Br_{ag} value for aboveground produce was obtained as follows: (1) Br_{ag} values for fruits combined with a human consumption rate of fruits of 1.44E-03 kg/kg/day, and (2) Br_{ag} values for vegetables combined with a human consumption rate of vegetables of 1.49E-03 kg/kg/day.	B-2-9	1.95E-02
Br_{forage} $(\frac{\mu g/g\ DW\ plant}{\mu g/g\ soil})$	Br_{forage} value was calculated by multiplying the uptake slope factor with a conversion factor of 2 x 10^9 g/ha soil. The uptake slope factor and the conversion factor were obtained from U.S. EPA (1992b) for leafy vegetables.	B-3-8	1.60E-02
Br_{grain} $(\frac{\mu g/g\ DW\ plant}{\mu g/g\ soil})$	Br_{grain} value was calculated by multiplying the uptake slope factors with a conversion factor of 2 x 10^9 g/ha soil. The uptake slope factor and the conversion factor were obtained from U.S. EPA (1992b) for grains/cereals.	B-3-8	2.00E-03
Bv_{ag} $(\frac{\mu g/g\ DW\ plant}{\mu g/g\ air})$	Metals are assumed to not experience air-to-leaf transfer, as cited in U.S. EPA (1995b).	B-2-8	NA

TABLE A-3-172

CHEMICAL-SPECIFIC INPUTS FOR SELENIUM (7782-49-2)

Parameter	Reference and Explanation	Equations	Value
Bv_{forage} $(\frac{\mu g/g\ DW\ plant}{\mu g/g\ air})$	Metals are assumed to not experience air-to-leaf transfer, as cited in U.S. EPA (1995b).	B-3-8	NA
Biotransfer Factors for Animals			
Ba_{milk} (day/kg FW)	Ba_{milk} values were obtained from U.S. EPA (1995a) for cadmium, selenium, and zinc. Values were calculated by dividing uptake slopes, as cited in U.S. EPA (1992b; 1995a), by a daily consumption rate of 20 kilograms dry weight per day and converting the result to a wet weight basis assuming a 87% moisture content in milk.	B-3-11	5.86E-03
Ba_{beef} (day/kg FW)	Ba_{beef} values were obtained from U.S. EPA (1995a) for cadmium, selenium, and zinc. Values were calculated by dividing uptake slopes, as cited in U.S. EPA (1992b; 1995a), by a daily consumption rate of 20 kilograms dry weight per day and converting the result to a wet weight basis assuming a 70% moisture content in beef.	B-3-10	2.27E-03
Ba_{pork} (day/kg FW)	Ba_{pork} values were obtained from U.S. EPA (1995a) for cadmium, selenium, and zinc. Values were calculated by dividing uptake slopes, as cited in U.S. EPA (1992b; 1995a), by a daily consumption rate of 4.7 kilograms dry weight per day and converting the result to a wet weight basis assuming a 70% moisture content in pork.	B-3-12	1.88E-01
Ba_{egg} (day/kg FW)	Ba_{egg} values were obtained from U.S. EPA (1995a) for cadmium, selenium, and zinc. Values were calculated by dividing uptake slopes, as cited in U.S. EPA (1992b; 1995a), by a daily consumption rate of 0.2 kilograms dry weight per day and converting the result to a wet weight basis assuming a 75% moisture content in eggs.	B-3-13	1.13E+00
$Ba_{chicken}$ (day/kg FW)	$Ba_{chicken}$ values were obtained from U.S. EPA (1995a) for cadmium, selenium, and zinc. Values were calculated by dividing uptake slopes, as cited in U.S. EPA (1992b; 1995a), by a daily consumption rate of 0.2 kilograms dry weight per day and converting the result to a wet weight basis assuming a 75% moisture content in chicken.	B-3-14	1.13E+00
BCF_{fish} (L/kg FW tissue)	Geometric mean value obtained from various literature sources (see Appendix A3.4).	B-4-26	1.29E+02
BAF_{fish} (L/kg FW)	--	B-4-27	NA
$BSAF_{fish}$ (unitless)	--	B-4-28	NA
Health Benchmarks			
RfD (mg/kg/day)	U.S. EPA (1997c)	C-1-8	5.0E-03
Oral *CSF* $(mg/kg/day)^{-1}$	--	C-1-7	ND
RfC (mg/m^3)	Calculated from *RfD* using an inhalation rate of 20 m^3/day and a human body weight of 70 kg.	C-2-3	1.8E-02

TABLE A-3-172

CHEMICAL-SPECIFIC INPUTS FOR SELENIUM (7782-49-2)

Parameter	Reference and Explanation	Equations	Value
Inhalation *URF* ($\mu g/m^3)^{-1}$	--	C-2-1	ND
Inhalation *CSF* $(mg/kg/day)^{-1}$	--	C-2-2	ND

Note:

All parameters are defined in list of FATE AND TRANSPORT PARAMETERS on page A-3-iii.

TABLE A-3-173

CHEMICAL-SPECIFIC INPUTS FOR SILVER (7440-22-4)

Parameter	Reference and Explanation	Equations	Value
Chemical/Physical Properties			
MW (g/mole)	Budavari, O'Neil, Smith, and Heckelman (1989)	--	107.87
T_m (^{o}K)	Budavari, O'Neil, Smith, and Heckelman (1989)	--	1,233.6
Vp (atm)	All metals, except mercury, are assumed to be nonvolatile at ambient temperatures.	--	0.0
S (mg/L)	All metals, except mercury, are assumed to be insoluble in water.	--	0.0
H (atm·m^3/mol)	*H* value is assumed to be zero, because the *Vp* and *S* values are zero for all metals, except mercury.	B-1-6; B-2-6; B-2-8; B-3-6; B-4-6; B-4-12; B-4-19	0.0
D_a (cm^2/s)	D_a value was calculated using the equation cited in U.S. EPA (1996a).	B-1-6; B-2-6; B-3-6; B-4-6; B-4-21	8.38E-02
D_w (cm^2/s)	D_w value was calculated using the equation cited in U.S. EPA (1996a).	B-4-20	9.71E-06
K_{ow} (unitless)	--	--	NA
K_{oc} (mL/g)	--	--	NA
Kd_s (mL/g)	Kd_s value was obtained from U.S. EPA (1996a), which provides pH-based values that were estimated by using the MINTEQ2 geochemical speciation model.	B-1-3; B-1-4; B-1-5; B-1-6; B-2-3; B-2-4; B-2-5; B-2-6; B-2-10; B-3-3; B-3-4; B-3-5; B-3-6; B-4-3; B-4-4; B-4-5; B-4-6; B-4-10; B-4-11	0.1 at pH=4.9; 8.3 at pH=6.8; 110 at pH=8.0
Kd_{sw} (L/Kg)	Kd_{sw} value is assumed to be same as the Kd_s value, because organic carbon does not play a major role in sorption for the metals, as cited in U.S. EPA (1994f).	B-4-16; B-4-18; B-4-24	0.1 at pH=4.9; 8.3 at pH=6.8; 110 at pH=8.0
Kd_{bs} (mL/g)	Kd_{bs} value is assumed to be same as the Kd_s value, because organic carbon does not play a major role in sorption for the metals, as cited in U.S. EPA (1994f).	B-4-16; B-4-25	0.1 at pH=4.9; 8.3 at pH=6.8; 110 at pH=8.0
ksg (year)$^{-1}$	--	B-1-2; B-2-2; B-3-2; B-4-2	ND

TABLE A-3-173

CHEMICAL-SPECIFIC INPUTS FOR SILVER (7440-22-4)

Parameter	Reference and Explanation	Equations	Value
Chemical/Physical Properties (Continued)			
Fv (unitless)	Because they are nonvolatile, metals are assumed to be 100 percent in particulate phase and zero percent in the vapor phase, as cited in U.S. EPA (1994f).	B-1-1; B-2-1; B-2-7; B-2-8; B-3-1; B-3-7; B-3-8; B-4-1; B-4-8; B-4-9; B-4-12; B-5-1	0.0
Biotransfer Factors for Plants			
RCF $(\frac{\mu g/g\ DW\ plant}{\mu g/mL\ soil\ water})$	--	B-2-10	ND
$Br_{rootveg}$ $(\frac{\mu g/g\ DW\ plant}{\mu g/g\ soil})$	$Br_{rootveg}$ value was obtained from Baes, Sharp, Sjoreen, and Shor (1984). *Br* values for nonvegetative growth (such as tubers) in Baes, Sharp, Sjoreen, and Shor (1984) were used for $Br_{root\ veg}$.	B-2-10	1.00E-01
Br_{ag} $(\frac{\mu g/g\ DW\ plant}{\mu g/g\ soil})$	Br_{ag} value for fruits was obtained from Baes, Sharp, Sjoreen, and Shor (1984). *Br* values for nonvegetative growth (reproductive) in Baes, Sharp, Sjoreen, and Shor (1984) were used for Br_{ag} (fruits). Br_{ag} value for vegetables was calculated using data obtained from Baes, Sharp, Sjoreen, and Shor (1984). *Br* values for nonvegetative (reproductive) growth and *Bv* values for vegetative growth weighted as 75% (reproductive) and 25% vegetative (Baes, Sharp, Sjoreen, and Shor [1984])—were used for Br_{ag} (vegetables). The weighted average Br_{ag} value for aboveground produce was obtained as follows: (1) Br_{ag} values for fruits combined with a human consumption rate of fruits of 1.44E-03 kg/kg/day, and (2) Br_{ag} values for vegetables combined with a human consumption rate of vegetables of 1.49E-03 kg/kg/day.	B-2-9	1.38E-01
Br_{forage} $(\frac{\mu g/g\ DW\ plant}{\mu g/g\ soil})$	Br_{forage} value was obtained from Baes, Sharp, Sjoreen, and Shor (1984). *Bv* values for vegetative growth (such as leaves and stems) in Baes, Sharp, Sjoreen, and Shor (1984) were used for Br_{forage}.	B-3-8	4.00E-01
Br_{grain} $(\frac{\mu g/g\ DW\ plant}{\mu g/g\ soil})$	Br_{grain} value was obtained from Baes, Sharp, Sjoreen, and Shor (1984). *Br* values for nonvegetative growth as recommended by Baes, Sharp, Sjoreen, and Shor (1984) were used for Br_{grain}.	B-3-8	1.00E-01
Bv_{ag} $(\frac{\mu g/g\ DW\ plant}{\mu g/g\ air})$	Metals are assumed to not experience air-to-leaf transfer, as cited in U.S. EPA (1995b).	B-2-8	NA

TABLE A-3-173

CHEMICAL-SPECIFIC INPUTS FOR SILVER (7440-22-4)

Parameter	Reference and Explanation	Equations	Value
Biotransfer Factors for Plants (Continued)			
Bv_{forage} $(\frac{\mu g/g\ DW\ plant}{\mu g/g\ air})$	Metals are assumed not to experience air-to-leaf transfer, as cited in U.S. EPA (1995b).	B-3-8	NA
Biotransfer Factors for Animals			
Ba_{milk} (day/kg FW)	Ba_{milk} values were obtained from Baes, Sharp, Sjoreen, and Shor (1984) for all metals, except cadmium, mercury, selenium, and zinc.	B-3-11	2.0E-02
Ba_{beef} (day/kg FW)	Ba_{beef} values were obtained from Baes, Sharp, Sjoreen, and Shor (1984) for all metals, except cadmium, mercury, selenium, and zinc.	B-3-10	3.0E-03
Ba_{pork} (day/kg FW)	NC DEHNR (1997)	B-3-12	ND
Ba_{egg} (day/kg FW)	--	B-3-13	ND
$Ba_{chicken}$ (day/kg FW)	--	B-3-14	ND
BCF_{fish} (L/kg FW tissue)	Geometric mean value obtained from various literature sources (see Appendix A3.4).	B-4-26	2.04E+02
BAF_{fish} (L/kg FW)	--	B-4-27	NA
$BSAF_{fish}$ (unitless)	--	B-4-28	NA
Health Benchmarks			
RfD (mg/kg/day)	U.S. EPA (1997b)	C-1-8	5.0E-03
Oral CSF $(mg/kg/day)^{-1}$	--	C-1-7	ND
RfC (mg/m^3)	Calculated from *RfD* using an inhalation rate of 20 m^3/day and a human body weight of 70 kg.	C-2-3	1.80E-02
Inhalation URF $(\mu g/m^3)^{-1}$	--	C-2-1	ND
Inhalation CSF $(mg/kg/day)^{-1}$	--	C-2-2	ND

Note:

All parameters are defined in list of FATE AND TRANSPORT PARAMETERS on page A-3-iii.

TABLE A-3-174

CHEMICAL-SPECIFIC INPUTS FOR STRYCHNINE (57-24-9)

Parameter	Reference and Explanation	Equations	Value
Chemical/Physical Properties			
MW (g/mole)	Budavari, O'Neil, Smith, and Heckelman (1989)	--	334.40
T_m (K)	Budavari, O'Neil, Smith, and Heckelman (1989)	--	541.1
Vp (atm)	*Vp* value cited in U.S. EPA (1995b).	--	2.20E-13 at 25°C (solid)
S (mg/L)	Montgomery and Welkom (1991)	--	1.50E+02
H (atm·m^3/mol)	*H* value was calculated by using the theoretical equation from Lyman, Reehl, and Rosenblatt (1982), which defines the constant. Recommended value was calculated by using the *MW*, *S*, and *Vp* values that are provided in this table.	B-1-6; B-2-6; B-2-8; B-3-6; B-4-6; B-4-12; B-4-19	4.90E-13
D_a (cm^2/s)	D_a value was obtained from CHEMDAT8 database (U.S. EPA 1994d).	B-1-6; B-2-6; B-3-6; B-4-6; B-4-21	1.38E-02
D_w (cm^2/s)	D_w value was obtained from CHEMDAT8 database (U.S. EPA 1994d).	B-4-20	5.58E-06
K_{ow} (unitless)	Arithmetic mean value cited in Karickhoff and Long (1995).	--	8.51E+01
K_{oc} (mL/g)	K_{oc} value was calculated by using the correlation equation with K_{ow} for all nonionizing organics except phthalates, PAHs, dioxins, and furans as cited in U.S. EPA (1994c). K_{oc} value was calculated by using the recommended K_{ow} value that is provided in this table.	--	4.53E+02
Kd_s (cm^3/g)	Kd_s value was calculated by using the correlation equation with K_{oc} that is cited in U.S. EPA (1993d) for an assumed organic carbon fraction of 0.01 in soil. Measured organic carbon in soil, specific to site conditions, should be used to calculate Kd_s, because the value varies, depending on the fraction of organic carbon in soil. Recommended Kd_s value was calculated by using the K_{oc} value that is provided in this table.	B-1-3; B-1-4; B-1-5; B-1-6; B-2-3; B-2-4; B-2-5; B-2-6; B-2-10; B-3-3; B-3-4; B-3-5; B-3-6; B-4-3; B-4-4; B-4-5; B-4-6; B-4-10; B-4-11	4.53E-01
Kd_{sw} (L/Kg)	Kd_{sw} value was calculated by using the correlation equation with K_{oc} that is cited in U.S. EPA (1993d) for an assumed organic carbon fraction of 0.075 in suspended sediment. Measured organic carbon in suspended sediment, specific to site conditions, should be used to calculate Kd_{sw}, because the value varies, depending on the fraction of organic carbon in suspended sediment. Recommended Kd_{sw} value was calculated by using the K_{oc} value that is provided in this table.	B-4-16; B-4-18; B-4-24	3.40E+00
Kd_{bs} (cm^3/g)	Kd_{bs} value was calculated by using the correlation equation with K_{oc} that is cited in U.S. EPA (1993d) for an assumed organic carbon fraction of 0.04 in bottom sediment. Measured organic carbon in bottom sediment, specific to site conditions, should be used to calculate Kd_{bs}, because the value varies depending on the fraction of organic carbon in bottom sediment. Recommended Kd_{bs} value was calculated by using the K_{oc} value that is provided in this table.	B-4-16; B-4-25	1.81E+00

TABLE A-3-174

CHEMICAL-SPECIFIC INPUTS FOR STRYCHNINE (57-24-9)

Parameter	Reference and Explanation	Equations	Value
Chemical/Physical Properties (Continued)			
ksg $(year)^{-1}$	*Ksg* value was calculated by using the chemical half-life in soil, as cited in Howard, Boethling, Jarvis, Meylan, and Michalenko (1991)	B-1-2; B-2-2; B-3-2; B-4-2	9.03E+00
Fv (unitless)	*Fv* value was calculated by using equations cited in Junge (1977) and Bidleman (1988). Recommended value of *Fv* was calculated by using S, T_m, and *Vp* values that are provided in this table. *Vp* value for this compound was converted to a liquid-phase value before being used in the calculations.	B-1-1; B-2-1; B-2-7; B-2-8; B-3-1; B-3-7; B-3-8; B-4-1; B-4-8; B-4-9; B-4-12; B-5-1	0.086
Biotransfer Factors for Plants			
RCF $(\frac{\mu g/g\ DW\ plant}{\mu g/mL\ soil\ water})$	*RCF* value was calculated by using the correlation equation with K_{ow} that is cited in Briggs (1982). Recommended value was calculated by using the K_{ow} value that is provided in this table. The value was then converted to a dry weight basis using a moisture content of 87 percent.	B-2-10	1.34E+01
$Br_{root\ veg}$ $(\frac{\mu g/g\ DW\ plant}{\mu g/g\ soil})$	$Br_{root\ veg}$ value was calculated by dividing the *RCF* value with the *Kds* value provided in this table (see section A4.3.2 of Appendix A-3).	B-2-10	2.96E+01
Br_{ag} $(\frac{\mu g/g\ DW\ plant}{\mu g/g\ soil})$	Br_{ag} value was calculated by using the correlation equation with K_{ow} that is cited in Travis and Arms (1988). No distinction was made between values for aboveground produce and forage. Recommended value was calculated by using the K_{ow} value that is provided in this table.	B-2-9	2.97E+00
Br_{forage} $(\frac{\mu g/g\ DW\ plant}{\mu g/g\ soil})$	Br_{forage} value was calculated by using the correlation equation with K_{ow} that is cited in Travis and Arms (1988). No distinction was made between values for aboveground produce and forage. Recommended value was calculated by using the K_{ow} value that is provided in this table.	B-3-9	2.97E+00
Bv_{ag} $(\frac{\mu g/g\ DW\ plant}{\mu g/g\ air})$	Bv_{ag} value was calculated by using the correlation equation with K_{ow} and *H* that is cited in Bacci, Calamari, Gaggi, and Vighi (1990); and Bacci, Cerejeira, Gaggi, Chemello, Calamari, and Vight (1992); then reducing this value by a factor of 100, as recommended by U.S. EPA (1993d). No distinction was made between values for aboveground produce and forage. Recommended value was calculated, for a temperature (T) of 25°C, by using the H and K_{ow} values that are provided in this table.	B-2-8	1.29E+07
Bv_{forage} $(\frac{\mu g/g\ DW\ plant}{\mu g/g\ air})$	Bv_{forage} value was calculated by using the correlation equation with K_{ow} and *H* that is cited in Bacci, Calamari, Gaggi, and Vighi (1990); and Bacci, Cerejeira, Gaggi, Chemello, Calamari, and Vight (1992); then reducing this value by a factor of 100, as recommended by U.S. EPA (1993d). No distinction was made between values for aboveground produce and forage. Recommended value was calculated, for a temperature (T) of 25°C, by using the *H* and K_{ow} values that are provided in this table.	B-3-8	1.29E+07

TABLE A-3-174

CHEMICAL-SPECIFIC INPUTS FOR STRYCHNINE (57-24-9)

Parameter	Reference and Explanation	Equations	Value
Biotransfer Factors for Animals			
Ba_{milk} (day/kg FW)	Ba_{milk} value was calculated by using the correlation equation with K_{ow} that is cited in Travis and Arms (1988). Recommended value was calculated by using the K_{ow} value that is provided in this table.	B-3-11	6.76E-07
Ba_{beef} (day/kg FW)	Ba_{beef} value was calculated by using the correlation equation with K_{ow} that is cited in Travis and Arms (1988). Recommended value was calculated by using the K_{ow} value that is provided in this table.	B-3-10	2.14E-06
Ba_{pork} (day/kg FW)	Ba_{pork} value was calculated by using thethe fat content ratio of pork to beef (23/19) and multiplying it with the Ba_{beef} value (see section A4.3.2 of Appendix A-3).	B-3-12	2.59E-06
Ba_{eggs} (day/kg FW)	Ba_{eggs} value was calculated by using the correlation equation with K_{ow} that is cited in California EPA (1993). Recommended value was calculated by using the K_{ow} value that is provided in this table.	B-3-13	6.76E-04
$Ba_{chicken}$ (day/kg FW)	$Ba_{chicken}$ value was calculated by using the fat content ratio of chicken to beef (15/19) and multiplying it with the Ba_{beef} value (see section A4.3.3 of Appendix A-3).	B-3-14	1.69E-06
BCF_{fish} (L/kg, FW tissue)	*BCFs* were used for compounds with a log K_{ow} value below 4.0, as cited in U.S. EPA (1995b). BCF_{fish} value calculated using the correlation equation with K_{ow} obtained from Veith, Macek, Petrocelli, and Caroll (1980)—See Appendix A-3.	B-4-26	1.72E+01
BAF_{fish} (L/kg FW)	--	B-4-27	NA
$BSAF_{fish}$ (unitless)	--	B-4-28	NA
Health Benchmarks			
RfD (mg/kg/day)	U.S. EPA (1997b)	C-1-8	3.0E-04
Oral CSF $(mg/kg/day)^{-1}$	--	C-1-7	ND
RfC (mg/m^3)	Calculated from *RfD* using an inhalation rate of 20 m^3/day and a human body weight of 70kg.	C-2-3	1.1E-03
Inhalation URF $(\mu g/m^3)^{-1}$	---	C-2-1	ND
Inhalation CSF $(mg/kg/day)^{-1}$	--	C-2-2	ND

Note:

NA = Note applicable
ND = No data available

All parameters are defined in list of FATE AND TRANSPORT PARAMETERS on page A-3-iii.

TABLE A-3-175

CHEMICAL-SPECIFIC INPUTS FOR STYRENE (100-42-5)

Parameter	Reference and Explanation	Equations	Value
Chemical/Physical Properties			
MW (g/mole)	Budavari, O'Neil, Smith, and Heckelman (1989)	--	104.14
T_m (K)	Budavari, O'Neil, Smith, and Heckelman (1989)	--	242.5
Vp (atm)	Geometric mean value cited in U.S. EPA (1994c).	--	8.21E-03 at 25°C (liquid)
S (mg/L)	Geometric mean value cited in U.S. EPA (1994c).	--	2.57E+02
H (atm·m^3/mol)	*H* value was calculated by using the theoretical equation from Lyman, Reehl, and Rosenblatt (1982), which defines the constant. Recommended value was calculated by using the *MW*, *S*, and *Vp* values that are provided in this table.	B-1-6; B-2-6; B-2-8; B-3-6; B-4-6; B-4-12; B-4-19	3.33E-03
D_a (cm^2/s)	D_a value was obtained from CHEMDAT8 database (U.S. EPA 1994d).	B-1-6; B-2-6; B-3-6; B-4-6; B-4-21	7.73E-02
D_w (cm^2/s)	D_w value was obtained from CHEMDAT8 database (U.S. EPA 1994d).	B-4-20	8.77E-06
K_{ow} (unitless)	Geometric mean value cited in U.S. EPA (1994c).	--	8.49E+02
K_{oc} (mL/g)	Geometric mean of measured values obtained from U.S. EPA (1996b).	--	9.12E+02
Kd_s (cm^3/g)	Kd_s value was calculated by using the correlation equation with K_{oc} that is cited in U.S. EPA (1993d) for an assumed organic carbon fraction of 0.01 in soil. Measured organic carbon in soil, specific to site conditions, should be used to calculate Kd_s, because the value varies, depending on the fraction of organic carbon in soil. Recommended Kd_s value was calculated by using the K_{oc} value that is provided in this table.	B-1-3; B-1-4; B-1-5; B-1-6; B-2-3; B-2-4; B-2-5; B-2-6; B-2-10; B-3-3; B-3-4; B-3-5; B-3-6; B-4-3; B-4-4; B-4-5; B-4-6; B-4-10; B-4-11	9.12E+00
Kd_{sw} (L/Kg)	Kd_{sw} value was calculated by using the correlation equation with K_{oc} that is cited in U.S. EPA (1993d) for an assumed organic carbon fraction of 0.075 in suspended sediment. Measured organic carbon in suspended sediment, specific to site conditions, should be used to calculate Kd_{sw}, because the value varies, depending on the fraction of organic carbon in suspended sediment. Recommended Kd_{sw} value was calculated by using the K_{oc} value that is provided in this table.	B-4-16; B-4-18; B-4-24	6.84E+01
Kd_{bs} (cm^3/g)	Kd_{bs} value was calculated by using the correlation equation with K_{oc} that is cited in U.S. EPA (1993d) for an assumed organic carbon fraction of 0.04 in bottom sediment. Measured organic carbon in bottom sediment, specific to site conditions, should be used to calculate Kd_{bs}, because the value varies, depending on the fraction of organic carbon in bottom sediment. Recommended Kd_{bs} value was calculated by using the K_{oc} value that is provided in this table.	B-4-16; B-4-25	3.65E+01
Chemical/Physical Properties (Continued)			
ksg (year)$^{-1}$	*ksg* value was calculated by using the chemical half-life in soil, as cited in Howard, Boethling, Jarvis, Meylan, and Michalenko (1991).	B-1-2; B-2-2; B-3-2; B-4-2	9.03E+00
Fv (unitless)	*Fv* value was calculated by using the equation cited in Junge (1977). Recommended value of *Fv* was calculated by using the *Vp* value that is provided in this table.	B-1-1; B-2-1; B-2-7; B-2-8; B-3-1; B-3-7; B-3-8; B-4-1;	1.0

TABLE A-3-175

CHEMICAL-SPECIFIC INPUTS FOR STYRENE (100-42-5)

Parameter	Reference and Explanation	Equations	Value
Biotransfer Factors for Plants			
RCF $(\frac{\mu g/g\ DW\ plant}{\mu g/mL\ soil\ water})$	*RCF* value was calculated by using the correlation equation with K_{ow} that is cited in Briggs (1982). Recommended value was calculated by using the K_{ow} value that is provided in this table. The value was then converted to a dry weight basis by using a moisture content of 87 percent.	B-2-10	4.81E+01
$Br_{root\ veg}$ $(\frac{\mu g/g\ DW\ plant}{\mu g/g\ soil})$	$Br_{root\ veg}$ value was calculated by dividing the *RCF* value with the Kd_s value provided in this table.	B-2-10	5.28E+00
Br_{ag} $(\frac{\mu g/g\ DW\ plant}{\mu g/g\ soil})$	Br_{ag} value was calculated by using the correlation equation with K_{ow} that is cited in Travis and Arms (1988). No distinction was made between values for aboveground produce and forage. Recommended value was calculated by using the K_{ow} value that is provided in this table.	B-2-9	7.85E-01
Br_{forage} $(\frac{\mu g/g\ DW\ plant}{\mu g/g\ soil})$	Br_{forage} value was calculated by using the correlation equation with K_{ow} that is cited in Travis and Arms (1988). No distinction was made between values for abovegroud produce and forage. Recommended value was calculated by using the K_{ow} value that is provided in this table.	B-3-9	7.85E-01
Bv_{ag} $(\frac{\mu g/g\ DW\ plant}{\mu g/g\ air})$	Bv_{ag} value was calculated by using the correlation equation with K_{ow} and *H* that is cited in Bacci, Calamari, Gaggi, and Vighi (1990); and Bacci, Cerejeira, Gaggi, Chemello, Calamari, and Vighi (1992); then reducing this value by a factor of 100. No distinction was made between values for aboveground produce and forage. Recommended value was calculated, for a temperature (T) of 25ºC, by using the *H* and K_{ow} values that are provided in this table.	B-2-8	2.21E-02
Bv_{forage} $(\frac{\mu g/g\ DW\ plant}{\mu g/g\ air})$	Bv_{forage} value was calculated by using the correlation equation with K_{ow} and *H* that is cited in Bacci, Calamari, Gaggi, and Vighi (1990); and Bacci, Cerejeira, Gaggi, Chemello, Calamari, and Vighi (1992); then reducing this value by a factor of 100. No distinction was made between values for aboveground produce and forage. Recommended value was calculated, for a temperature (T) of 25ºC, by using the *H* and K_{ow} values that are provided in this table.	B-3-8	2.21E-02
Biotransfer Factors for Animals			
Ba_{milk} (day/kg FW)	Ba_{milk} value was calculated by using the correlation equation with K_{ow} that is cited in Travis and Arms (1988). Recommended value was calculated by using the K_{ow} value that is provided in this table.	B-3-11	6.74E-06
Ba_{beef} (day/kg FW)	Ba_{beef} value was calculated by using the correlation equation with K_{ow} that is cited in Travis and Arms (1988). Recommended value was calculated by using the K_{ow} value that is provided in this table.	B-3-10	2.13E-05
Ba_{pork} (day/kg FW)	Ba_{pork} value was calculated by using the fat content ratio of pork to beef (23/19) and multiplying it with the Ba_{beef} value.	B-3-12	2.58E-05
Ba_{eggs} (day/kg FW)	Ba_{eggs} value was calculated by using the correlation equation with K_{ow} that is cited in California EPA (1993). Recommended value was calculated by using the K_{ow} value that is provided in this table.	B-3-13	6.74E-03
$Ba_{chicken}$ (day/kg FW)	$Ba_{chicken}$ value was calculated by using the fat content ratio of chicken to beef (15/19) and multiplying it with the Ba_{beef} value.	B-3-14	1.68E-05

TABLE A-3-175

CHEMICAL-SPECIFIC INPUTS FOR STYRENE (100-42-5)

Parameter	Reference and Explanation	Equations	Value
BCF_{fish} (L/kg FW tissue)	*BCFs* were used for compounds with a log K_{ow} value below 4.0, as cited in U.S. EPA (1995b). BCF_{fish} value calculated using the correlation equation with K_{ow} obtained from Veith, Macek, Petrocelli, and Caroll (1980)—See Appendix A-3.	B-4-26	9.91E+01
BAF_{fish} (L/kg FW)	--	B-4-27	NA
$BSAF_{fish}$ (unitless)	--	B-4-28	NA
Health Benchmarks			
RfD (mg/kg/day)	U.S. EPA (1997b)	C-1-8	2.0E-01
Oral CSF $(mg/kg/day)^{-1}$	--	C-1-7	ND
RfC (mg/m^3)	U.S. EPA (1997b)	C-2-3	1.0E+00
Inhalation URF $(\mu g/m^3)^{-1}$	--	C-2-1	ND
Inhalation CSF $(mg/kg/day)^{-1}$	--	C-2-2	ND

Note:

NA = Not applicable
ND = No data available

All parameters are defined in list of FATE AND TRANSPORT PARAMETERS on page A-3-iii.

TABLE A-3-176

CHEMICAL-SPECIFIC INPUTS FOR 2,3,7,8-TETRACHLORODIBENZO(P)DIOXIN (1746-01-6)

Parameter	Reference and Explanation	Equations	Value
Chemical/Physical Properties			
MW (g/mole)	U.S. EPA (1994a)	--	321.98
T_m (K)	U.S. EPA (1994a)	--	578.1
Vp (atm)	U.S. EPA (1994a)	--	4.45E-11 at 25°C (solid)
S (mg/L)	U.S. EPA (1994a)	--	4.83E-04
H (atm·m^3/mol)	U.S. EPA (1994a)	B-1-6; B-2-6; B-2-8; B-3-6; B-4-6; B-4-12; B-4-19	1.60E-05
D_a (cm^2/s)	D_a value was obtained from CHEMDAT8 database (U.S. EPA 1994d).	B-1-6; B-2-6; B-3-6; B-4-6; B-4-21	1.27E-02
D_w (cm^2/s)	D_w value was obtained from CHEMDAT8 database (U.S. EPA 1994d).	B-4-20	6.81E-06
K_{ow} (unitless)	U.S. EPA (1994a)	--	4.37E+06
K_{oc} (mL/g)	K_{oc} value was calculated by using the correlation equation with K_{ow} for dioxins and furans that is cited in U.S. EPA (1994a; 1994b). Recommended value was calculated by using the recommended K_{ow} value that is provided in this table.	--	2.69E+04
Kd_s (mL/g)	Kd_s value was calculated by using the correlation equation with K_{oc} that is cited in U.S. EPA (1993d) for an assumed organic carbon fraction of 0.01 in soil. Measured organic carbon in soil, specific to site conditions, should be used to calculate Kd_s, because the value varies, depending on the fraction of organic carbon in soil. Recommended Kd_s value was calculated by using the K_{oc} value that is provided in this table.	B-1-3; B-1-4; B-1-5; B-1-6; B-2-3; B-2-4; B-2-5; B-2-6; B-2-10; B-3-3; B-3-4; B-3-5; B-3-6; B-4-3; B-4-4; B-4-5; B-4-6; B-4-10; B-4-11	2.69E+04
Kd_{sw} (L/Kg)	Kd_{sw} value was calculated by using the correlation equation with K_{oc} that is cited in U.S. EPA (1993d) for an assumed organic carbon fraction of 0.075 in suspended sediment. Measured organic carbon in suspended sediment, specific to site conditions, should be used to calculate Kd_{sw}, because the value varies, depending on the fraction of organic carbon in suspended sediment. Recommended Kd_{sw} value was calculated by using the K_{oc} value that is provided in this table.	B-4-16; B-4-18; B-4-24	2.02E+05
Kd_{bs} (mL/g)	Kd_{bs} value was calculated by using the correlation equation with K_{oc} that is cited in U.S. EPA (1993d) for an assumed organic carbon fraction of 0.04 in bottom sediment. Measured organic carbon in bottom sediment, specific to site conditions, should be used to calculate Kd_{bs}, because the value varies, depending on the fraction of organic carbon in bottom sediment. Recommended Kd_{bs} value was calculated by using the K_{oc} value that is provided in this table.	B-4-16; B-4-25	1.08E+05
Chemical/Physical Properties (Continued)			
ksg (year)$^{-1}$	*ksg* value was calculated by using the chemical half-life in soil, as cited in Mackay, Shiu, and Ma (1992).	B-1-2; B-2-2; B-3-2; B-4-2	4.29E-01

TABLE A-3-176

CHEMICAL-SPECIFIC INPUTS FOR 2,3,7,8-TETRACHLORODIBENZO(P)DIOXIN (1746-01-6)

Parameter	Reference and Explanation	Equations	Value
Fv (unitless)	*Fv* value was calculated by using equations cited in Junge (1977) and Bidleman (1988). Recommended value of *Fv* was calculated by using *S*, T_m, and *Vp* values that are provided in this table. *Vp* value for this compound was converted to a liquid phase value before being used in the calculations.	B-1-1; B-2-1; B-2-7; B-2-8; B-3-1; B-3-7; B-3-8; B-4-1; B-4-8; B-4-9; B-4-12; B-5-1	9.78E-01
Biotransfer Factors for Plants			
RCF $(\frac{\mu g/g\ DW\ plant}{\mu g/mL\ soil\ water})$	*RCF* value was calculated by using the correlation equation with K_{ow} that is cited in Briggs (1982). Recommended value was calculated by using the K_{ow} value that is provided in this table. The value was then converted to a dry weight basis by using a moisture content of 87 percent.	B-2-10	3.01E+04
$Br_{root\ veg}$ $(\frac{\mu g/g\ DW\ plant}{\mu g/g\ soil})$	$Br_{root\ veg}$ value was calculated by dividing the *RCF* value with the Kd_s value provided in this table.	B-2-10	1.12E+00
Br_{ag} $(\frac{\mu g/g\ DW\ plant}{\mu g/g\ soil})$	Br_{ag} value was calculated by using the correlation equation with K_{ow} that is cited in Travis and Arms (1988). No distinction was made between values for aboveground produce and forage. Recommended value was calculated by using the K_{ow} value that is provided in this table.	B-2-9	5.62E-03
Br_{forage} $(\frac{\mu g/g\ DW\ plant}{\mu g/g\ soil})$	Br_{forage} value was calculated by using the correlation equation with K_{ow} that is cited in Travis and Arms (1988). No distinction was made between values for aboveground produce and forage. Recommended value was calculated by using the K_{ow} value that is provided in this table.	B-3-9	5.62E-03
Bv_{ag} $(\frac{\mu g/g\ DW\ plant}{\mu g/g\ air})$	Bv_{ag} value was obtained from Lorber (1995). No distinction was made between aboveground produce and forage.	B-2-8	6.10E+04
Bv_{forage} $(\frac{\mu g/g\ DW\ plant}{\mu g/g\ air})$	Bv_{forage} value was obtained from Lorber (1995). No distinction was made between aboveground produce and forage.	B-3-8	6.10E+04
Biotransfer Factors for Animals			
Ba_{milk} (day/kg FW)	U.S. EPA (1995a)	B-3-11	1.00E-02
Ba_{beef} (day/kg FW)	Ba_{beef} value was calculated by increasing Ba_{milk} values by a factor of 5.43, as discussed in Section A3.3.14.	B-3-10	5.43E-02
Ba_{pork} (day/kg FW)	Ba_{pork} value was calculated by increasing Ba_{milk} values by a factor of 6.57, as discussed in Section A3.3.15.	B-3-12	6.57E-02

TABLE A-3-176

CHEMICAL-SPECIFIC INPUTS FOR 2,3,7,8-TETRACHLORODIBENZO(P)DIOXIN (1746-01-6)

Parameter	Reference and Explanation	Equations	Value
Ba_{egg} (L/kg FW tissue)	Ba_{egg} value was calculated by multiplying the BCF value for chicken eggs by a chicken soil consumption rate of 0.02 kg (DW)/day (See Appendix A-3). BCF value for eggs was obtained from Stephens, Petreas, and Hayward (1995) for the high exposure chicken group.	B-3-13	5.42E-02
$Ba_{chicken}$ (L/kg FW tissue)	$Ba_{chickens}$ value was calculated by multiplying the BCF value for chicken by a chicken soil consumption rate of 0.02 kg (DW)/day (See Appendix A-3). BCF value for chicken was obtained from Stephens, Petreas, and Hayward (1995) for the high exposure chicken group.	B-3-14	7.30E-02
BCF_{fish} (L/kg FW tissue)	--	B-4-26	NA
BAF_{fish} (L/kg FW)	--	B-4-27	NA
$BSAF_{fish}$ (unitless, lipid based)	U.S. EPA (1994a)	B-4-28	9.00E-02
Other Parameters			
TEF (unitless)	U.S. EPA (1994a)	--	1.00
Health Benchmarks			
RfD (mg/kg/day)		C-1-8	ND
Oral CSF $(mg/kg/day)^{-1}$	U.S.EPA (1997c)	C-1-7	1.5E+05
RfC (mg/m^3)	--	C-2-3	ND
Inhalation URF $(\mu g/m^3)^{-1}$	U.S.EPA (1997c)	C-2-1	3.3E-08
Inhalation CSF $(mg/kg/day)^{-1}$	U.S.EPA (1997c)	C-2-2	1.5E+05

Note:

NA = Not Applicable; ND = No Data Available
All parameters are defined in in list of FATE AND TRANSPORT PARAMETERS on page A-3-iii.

TABLE A-3-177

CHEMICAL-SPECIFIC INPUTS FOR 2,3,7,8-TETRACHLORODIBENZO(P)FURAN (51207-31-9)

Parameter	Reference and Explanation	Equations	Value
Chemical/Physical Properties			
MW (g/mole)	U.S. EPA (1994a)	--	305.98
T_m (K)	U.S. EPA (1994a)	--	500.1
Vp (atm)	U.S. EPA (1994a)	--	1.97E-11 at 25°C (solid)
S (mg/L)	U.S. EPA (1994a)	--	4.19E-04
H (atm·m^3/mol)	U.S. EPA (1994a).	B-1-6; B-2-6; B-2-8; B-3-6; B-4-6; B-4-12; B-4-19	8.60E-06
D_a (cm^2/s)	D_a value was obtained from WATER8 model database (U.S. EPA 1995d).	B-1-6; B-2-6; B-3-6; B-4-6; B-4-21	1.79E-02
D_w (cm^2/s)	D_w value was calculated using the equation cited in U.S. EPA (1996a).	B-4-20	4.85E-06
K_{ow} (unitless)	U.S. EPA (1992d)	--	3.39E+06
K_{oc} (mL/g)	K_{oc} value was calculated by using the correlation equation with K_{ow} for dioxins and furans that is cited in U.S. EPA (1994a; 1994c). Recommended value was calculated by using the recommended K_{ow} value that is provided in this table.	--	2.09E+06
Kd_s (cm^3/g)	Kd_s value was calculated by using the correlation equation with K_{oc} that is cited in U.S. EPA (1993d) for an assumed organic carbon fraction of 0.01 in soil. Measured organic carbon in soil, specific to site conditions, should be used to calculate Kd_s, because the value varies, depending on the fraction of organic carbon in soil. Recommended Kd_s value was calculated by using the K_{oc} value that is provided in this table.	B-1-3; B-1-4; B-1-5; B-1-6; B-2-3; B-2-4; B-2-5; B-2-6; B-2-10; B-3-3; B-3-4; B-3-5; B-3-6; B-4-3; B-4-4; B-4-5; B-4-6; B-4-10; B-4-11	2.09E+04
Kd_{sw} (L/Kg)	Kd_{sw} value was calculated by using the correlation equation with K_{oc} that is cited in U.S. EPA (1993d) for an assumed organic carbon fraction of 0.075 in suspended sediment. Measured organic carbon in suspended sediment, specific to site conditions, should be used to calculate Kd_{sw}, because the value varies, depending on the fraction of organic carbon in suspended sediment. Recommended Kd_{sw} value was calculated by using the K_{oc} value that is provided in this table.	B-4-16; B-4-18; B-4-24	1.57E+05

TABLE A-3-177

CHEMICAL-SPECIFIC INPUTS FOR 2,3,7,8-TETRACHLORODIBENZO(P)FURAN (51207-31-9)

Parameter	Reference and Explanation	Equations	Value
Chemical/Physical Properties (Continued)			
Kd_{bs} (cm^3/g)	Kd_{bs} value was calculated by using the correlation equation with K_{oc} that is cited in U.S. EPA (1993d) for an assumed organic carbon fraction of 0.04 in bottom sediment. Measured organic carbon in bottom sediment, specific to site conditions, should be used to calculate Kd_{bs}, because the value varies depending on the fraction of organic carbon in bottom sediment. Recommended Kd_{bs} value was calculated by using the K_{oc} value that is provided in this table.	B-4-16; B-4-25	8.36E+04
ksg $(year)^{-1}$	*ksg* value was calculated by using the chemical half-life in soil, as cited in Mackay, Shiu, and Ma (1992).	B-1-1; B-1-2; B-2-1; B-2-2; B-3-1; B-3-2; B-4-1; B-4-2	3.57E-01
Fv (unitless)	*Fv* value was calculated by using equations cited in Junge (1977) and Bidleman (1988). Recommended value of Fv was calculated by using T_m and *Vp* values that are provided in this table. *Vp* value for this compound was converted to a liquid phase value before being used in the calculations.	B-1-1; B-2-1; B-2-7; B-2-8; B-3-1; B-3-7; B-3-8; B-4-1; B-4-8; B-4-9; B-4-12; B-5-1	7.68E-01
Biotransfer Factors for Plants			
RCF $(\frac{\mu g/g\ DW\ plant}{\mu g/mL\ soil\ water})$	*RCF* value was calculated by using the correlation equation with K_{ow} that is cited in Briggs (1982). Recommended value was calculated by using the K_{ow} value that is provided in this table. The value was then converted to a dry weight basis by using a moisture content of 87 percent.	B-2-10	2.48E+04
$Br_{rootveg}$ $(\frac{\mu g/g\ DW\ plant}{\mu g/g\ soil})$	$Br_{rootveg}$ value was calculated by dividing the *RCF* value with the Kd_s value provided in this table.	B-2-10	1.19E+00
Br_{ag} $(\frac{\mu g/g\ DW\ plant}{\mu g/g\ soil})$	Br_{ag} value was calculated by using the correlation equation with K_{ow} that is cited in Travis and Arms (1988). No distinction was made between values for aboveground produce and forage. Recommended value was calculated by using the K_{ow} value that is provided in this table.	B-2-9	6.51E-03
Br_{forage} $(\frac{\mu g/g\ DW\ plant}{\mu g/g\ soil})$	Br_{forage} value was calculated by using the correlation equation with K_{ow} that is cited in Travis and Arms (1988). No distinction was made between values for aboveground produce and forage. Recommended value was calculated by using the K_{ow} value that is provided in this table.	B-3-9	6.51E-03
Bv_{ag} $(\frac{\mu g/g\ DW\ plant}{\mu g/g\ air})$	Bv_{ag} value was obtained from Lorber (1995). No distinction was made between aboveground produce and forage.	B-2-8	8.10E+04

TABLE A-3-177

CHEMICAL-SPECIFIC INPUTS FOR 2,3,7,8-TETRACHLORODIBENZO(P)FURAN (51207-31-9)

Parameter	Reference and Explanation	Equations	Value
Biotransfer Factors for Plants (Continued)			
Bv_{forage} ($\frac{\mu g/g\ DW\ plant}{\mu g/g\ air}$)	Bv_{forage} value was obtained from Lorber (1995). No distinction was made between aboveground produce and forage.	B-3-8	8.10E+04
Biotransfer Factors for Animals			
Ba_{milk} (day/kg FW)	U.S. EPA (1995a)	B-3-11	3.00E-03
Ba_{beef} (day/kg FW)	Ba_{beef} value was calculated by increasing Ba_{milk} values by a factor of 5.43, as discussed in Section A3.3.14.	B-3-10	1.63E-02
Ba_{pork} (day/kg FW)	Ba_{pork} value was calculated by increasing Ba_{milk} values by a factor of 6.57, as discussed in Section A3.3.15.	B-3-12	1.97E-02
Ba_{egg} (L/kg FW tissue)	Ba_{egg} value was calculated by multiplying the BCF value for chicken eggs by a chicken soil consumption rate of 0.02 kg (DW)/day (See Appendix A-3). BCF value for eggs was obtained from Stephens, Petreas, and Hayward (1995) for the high exposure chicken group.	B-3-13	3.61E-02
$Ba_{chicken}$ (L/kg FW tissue)	$Ba_{chicken}$ value was calculated by multiplying the BCF value for chicken by a chicken soil consumption rate of 0.02 kg (DW)/day (See Appendix A-3). BCF value for chicken was obtained from Stephens, Petreas, and Hayward (1995) for the high exposure chicken group.	B-3-14	5.63E-02
BCF_{fish} (L/kg FW tissue)	--	B-4-26	NA
BAF_{fish} (L/kg FW)	--	B-4-27	NA
$BSAF_{fish}$ (unitless, lipid based)	U.S. EPA (1994a)	B-4-28	9.00E-02
Other Parameters			
TEF (unitless)	U.S. EPA (1994a)	--	0.10
Health Benchmarks			
Oral CSF $(mg/kg/day)^{-1}$	--	C-1-8	ND
Inhalation CSF $(mg/kg/day)^{-1}$	--	C-1-7	ND
RfD (mg/kg/day)	--	C-2-3	ND
Inhalation URF $(\mu g/m^3)^{-1}$	--	C-2-1	ND
RfC (mg/m^3)	--	C-2-2	ND

TABLE A-3-177

CHEMICAL-SPECIFIC INPUTS FOR 2,3,7,8-TETRACHLORODIBENZO(P)FURAN (51207-31-9)

Note:

NA = Not Applicable; ND = No Data Available
All parameters are defined in list of FATE AND TRANSPORT PARAMETERS on page A-3-iii.

TABLE A-3-178

CHEMICAL-SPECIFIC INPUTS FOR 1,2,4,5-TETRACHLOROBENZENE (95-94-3)

Parameter	Reference and Explanation	Equations	Value
Chemical/Physical Properties			
MW (g/mole)	Montgomery and Welkom (1991)	--	215.89
T_m (K)	Montgomery and Welkom (1991)	--	411.1
Vp (atm)	*Vp* value cited in U.S. EPA (1995b).	--	7.1E-06 at 25°C (solid)
S (mg/L)	*S* value cited in U.S. EPA (1995b).	--	1.30E+00
H (atm·m^3/mol)	*H* value was calculated by using the theoretical equation from Lyman, Reehl, and Rosenblatt (1982), which defines the constant. Recommended value was calculated by using the *MW*, *S*, and *Vp* values that are provided in this table.	B-1-6; B-2-6; B-2-8; B-3-6; B-4-6; B-4-12; B-4-19	1.18E-03
D_a (cm^2/s)	D_a value was obtained from CHEMDAT8 database (U.S. EPA 1994d).	B-1-6; B-2-6; B-3-6; B-4-6; B-4-21	2.11E-02
D_w (cm^2/s)	D_w value was obtained from CHEMDAT8 database (U.S. EPA 1994d).	B-4-20	8.75E-06
K_{ow} (unitless)	Arithmetic mean value cited in Karickhoff and Long (1995).	--	4.36E+04
K_{oc} (mL/g)	K_{oc} value was calculated by using the correlation equation with K_{ow} for all nonionizing organics except phthalates, PAHs, dioxins, and furans as cited in U.S. EPA (1994c). K_{oc} value was calculated by using the recommended K_{ow} value that is provided in this table.	--	5.89E+03
Kd_s (cm^3/g)	Kd_s value was calculated by using the correlation equation with K_{oc} that is cited in U.S. EPA (1993d) for an assumed fraction organic carbon of 0.01 in soil. Measured organic carbon in soil, specific to site conditions, should be used to calculate Kd_s, because the value varies, depending on the fraction of organic carbon in soil. Recommended Kd_s value was calculated by using the K_{oc} value that is provided in this table.	B-1-3; B-1-4; B-1-5; B-1-6; B-2-3; B-2-4; B-2-5; B-2-6; B-2-10; B-3-3; B-3-4; B-3-5; B-3-6; B-4-3; B-4-4; B-4-5; B-4-6; B-4-10; B-4-11	5.89E+01
Kd_{sw} (L/Kg)	Kd_{sw} value was calculated by using the correlation equation with K_{oc} that is cited in U.S. EPA (1993d) for an assumed organic carbon fraction of 0.075 in suspended sediment. Measured organic carbon in suspended sediment, specific to site conditions, should be used to calculate Kd_{sw}, because the value varies, depending on the fraction of organic carbon in suspended sediment. Recommended Kd_{sw} value was calculated by using the K_{oc} value that is provided in this table.	B-4-16; B-4-18; B-4-24	4.42E+02
Kd_{bs} (cm^3/g)	Kd_{bs} value was calculated by using the correlation equation with K_{oc} that is cited in U.S. EPA (1993d) for an assumed organic carbon of 0.04 in bottom sediment. Measured organic carbon in bottom sediment, specific to site conditions, should be used to calculate Kd_{bs}, because the value varies depending on the fraction of organic fraction in bottom sediment. Recommended Kd_{bs} value was calculated by using the K_{oc} value that is provided in this table.	B-4-16; B-4-25	2.36E+02

TABLE A-3-178

CHEMICAL-SPECIFIC INPUTS FOR 1,2,4,5-TETRACHLOROBENZENE (95-94-3)

Parameter	Reference and Explanation	Equations	Value
Chemical/Physical Properties (Continued)			
ksg $(year)^{-1}$	*ksg* value was calculated by using the chemical half-life in soil, as cited in Howard, Boethling, Jarvis, Meylan, and Michalenko (1991).	B-1-2; B-2-2; B-3-2; B-4-2	1.41E+00
Fv (unitless)	*Fv* value was calculated by using equations cited in Junge (1977) and Bidleman (1988). Recommended value of *Fv* was calculated by using *S*, T_m, and *Vp* values that are provided in this table. *Vp* value for this compound was converted to a liquid-phase value before being used in the calculations.	B-1-1; B-2-1; B-2-7; B-2-8; B-3-1; B-3-7; B-3-8; B-4-1; B-4-8; B-4-9; B-4-12; B-5-1	1.0
Biotransfer Factors for Plants			
RCF $(\frac{\mu g/g\ DW\ plant}{\mu g/mL\ soil\ water})$	*RCF* value was calculated by using the correlation equation with K_{ow} that is cited in Briggs (1982). Recommended value was calculated by using the K_{ow} value that is provided in this table. The value was converted to a dry weight basis by using a moisture content of 87 percent.	B-2-10	8.75E+02
$Br_{root\ veg}$ $(\frac{\mu g/g\ DW\ plant}{\mu g/g\ soil})$	$Br_{root\ veg}$ value was calculated by dividing the *RCF* value with the Kd_s value provided in this table.	B-2-10	1.49E+01
Br_{ag} $(\frac{\mu g/g\ DW\ plant}{\mu g/g\ soil})$	Br_{ag} value was calculated by using the correlation equation with K_{ow} that is cited in Travis and Arms (1988). No distinction was made between values for aboveground produce and forage. Recommended value was calculated by using the K_{ow} value that is provided in this table.	B-2-9	8.06E-02
Br_{forage} $(\frac{\mu g/g\ DW\ plant}{\mu g/g\ soil})$	Br_{forage} value was calculated by using the correlation equation with K_{ow} that is cited in Travis and Arms (1988). No distinction was made between values for aboveground produce and forage. Recommended value was calculated by using the K_{ow} value that is provided in this table.	B-3-9	8.06E-02
Bv_{ag} $(\frac{\mu g/g\ DW\ plant}{\mu g/g\ air})$	Bv_{ag} value was calculated by using the correlation equation with K_{ow} and *H* that is cited in Bacci, Calamari, Gaggi, and Vighi (1990); and Bacci, Cerejeira, Gaggi, Chemello, Calamari, and Vighi (1992); then reducing this value by a factor of 100, as recommended by U.S. EPA (1993d). No distinction was made between values for aboveground produce and forage. Recommended value was calculated, for a temperature (T) of 25°C, by using the *H* and K_{ow} values that are provided in this table.	B-2-8	4.14E+00
Bv_{forage} $(\frac{\mu g/g\ DW\ plant}{\mu g/g\ air})$	Bv_{forage} value was calculated by using the correlation equation with K_{ow} and *H* that is cited in Bacci, Calamari, Gaggi, and Vighi (1990); and Bacci, Cerejeira, Gaggi, Chemello, Calamari, and Vighi (1992); then reducing this value by a factor of 100, as recommended by U.S. EPA (1993d). No distinction was made between values for aboveground produce and forage. Recommended value was calculated, for a temperature (T) of 25°C, by using the *H* and K_{ow} values that are provided in this table.	B-3-8	4.14E+00
Biotransfer Factors for Animals			
Ba_{milk} (day/kg FW)	Ba_{milk} value was calculated by using the correlation equation with K_{ow} that is cited in Travis and Arms (1988). Recommended value was calculated by using the K_{ow} value that is provided in this table.	B-3-11	3.47E-04
Ba_{beef} (day/kg FW)	Ba_{beef} value was calculated by using the correlation equation with K_{ow} that is cited in Travis and Arms (1988). Recommended value was calculated by using the K_{ow} value that is provided in this table.	B-3-10	1.10E-03

TABLE A-3-178

CHEMICAL-SPECIFIC INPUTS FOR 1,2,4,5-TETRACHLOROBENZENE (95-94-3)

Parameter	Reference and Explanation	Equations	Value
Ba_{pork} (day/kg FW)	Ba_{pork} value was calculated by using the fat content ratio of pork to beef (23/19) and multiplying it with the Ba_{beef} value.	B-3-12	1.33E-03
Ba_{egg} (day/kg FW)	Ba_{egg} value was calculated by using the correlation equation with K_{ow} that is cited in California EPA (1993). Recommended value was calculated by using the K_{ow} value that is provided in this table.	B-3-13	3.47E-01
$Ba_{chicken}$ (day/kg FW)	$Ba_{chicken}$ value was calculated by using the fat content ratio of chicken to beef (15/19) and multiplying it with the Ba_{beef} value.	B-3-14	8.66E-04
BCF_{fish} (L/kg FW tissue)	--	B-4-26	NA
BAF_{fish} (L/kg FW)	*BAFs* were used for compounds with a log K_{ow} value above 4.0, as cited in U.S. EPA (1995b). *BAF* values were predicted values calculated by multiplying a food chain multiplier (*FCM*) with an estimated *BCF*. *BCF*s were estimated using the correlation equation obtained from Veith, Macek, Petrocelli, and Caroll (1980). *FCM*s were obtained from U.S. EPA (1995bc)—See Appendix A-3.	B-4-27	4.30E+03
$BSAF_{fish}$ (unitless)	--	B-4-28	NA
Health Benchmarks			
RfD (mg/kg/day)	U.S. EPA (1997b)	C-1-8	3.0E-04
Oral CSF $(mg/kg/day)^{-1}$	--	C-1-7	ND
RfC (mg/m^3)	Calculated from *RfD* using an inhalation rate of 20 m^3/day and a human body weight of 70 kg.	C-2-3	1.1E-03
Inhalation URF $(\mu g/m^3)^{-1}$	--	C-2-1	ND
Inhalation CSF $(mg/kg/day)^{-1}$	--	C-2-2	ND

Note:

NA= Not applicable
ND= No data available

All parameters are defined in list of FATE AND TRANSPORT PARAMETERS on page A-3-iii.

TABLE A-3-179

CHEMICAL-SPECIFIC INPUTS FOR 1,1,1,2-TETRACHLOROETHANE (630-20-6)

Parameter	Reference and Explanation	Equations	Value
Chemical/Physical Properties			
MW (g/mole)	Montgomery and Welkom (1991)	--	167.85
T_m (K)	Montgomery and Welkom (1991)	--	230.1
Vp (atm)	*Vp* value cited in U.S. EPA (1995b)	--	1.60E-02 at 25°C (liquid)
S (mg/L)	*S* value cited in U.S. EPA (1995b)	--	1.10E+03
H (atm·m^3/mol)	*H* value was calculated by using the theoretical equation from Lyman, Reehl, and Rosenblatt (1982), which defines the constant. Recommended value was calculated by using the *MW*, *S*, and *Vp* values that are provided in this table.	B-1-6; B-2-6; B-2-8; B-3-6; B-4-6; B-4-12; B-4-19	2.44E-03
D_a (cm^2/s)	D_a value was obtained from CHEMDAT8 database (U.S. EPA 1994d).	B-1-6; B-2-6; B-3-6; B-4-6; B-4-21	3.15E-02
D_w (cm^2/s)	D_w value was obtained from CHEMDAT8 database (U.S. EPA 1994d).	B-4-20	9.30E-06
K_{ow} (unitless)	Arithmetic mean value cited in Karickhoff and Long (1995)	--	4.27E+02
K_{oc} (mL/g)	K_{oc} value was calculated by using the correlation equation with K_{ow} for all nonionizing organics except phthalates, PAHs, dioxins, and furans, cited in U.S. EPA (1994c). K_{oc} value was calculated by using the recommended K_{ow} value that is provided in this table.	--	1.59E+02
Kd_s (cm^3/g)	Kd_s value was calculated by using the correlation equation with K_{oc} that is cited in U.S. EPA (1993d) for an assumed organic carbon fraction of 0.01 in soil. Measured organic carbon in soil, specific to site conditions, should be used to calculate Kd_s, because the value varies, depending on the fraction of organic carbon in soil. Recommended Kd_s value was calculated by using the K_{oc} value that is provided in this table.	B-1-3; B-1-4; B-1-5; B-1-6; B-2-3; B-2-4; B-2-5; B-2-6; B-2-10; B-3-3; B-3-4; B-3-5; B-3-6; B-4-3; B-4-4; B-4-5; B-4-6; B-4-10; B-4-11	1.59E+00
Kd_{sw} (L/Kg)	Kd_{sw} value was calculated by using the correlation equation with K_{oc} that is cited in U.S. EPA (1993d) for an assumed organic carbon fraction of 0.075 in suspended sediment. Measured organic carbon in suspended sediment, specific to site conditions, should be used to calculate Kd_{sw}, because the value varies, depending on the fraction of organic carbon in suspended sediment. Recommended Kd_{sw} value was calculated by using the K_{oc} value that is provided in this table.	B-4-16; B-4-18; B-4-24	1.20E+01
Kd_{bs} (cm^3/g)	Kd_{bs} value was calculated by using the correlation equation with K_{oc} that is cited in U.S. EPA (1993d) for an assumed organic carbon fraction of 0.04 in bottom sediment. Measured organic carbon in bottom sediment, specific to site conditions, should be used to calculate Kd_{bs}, because the value varies, depending on the fraction of organic carbon in bottom sediment. Recommended Kd_{bs} value was calculated by using the K_{oc} value that is provided in this table.	B-4-16; B-4-25	6.37E+00
Chemical/Physical Properties (Continued)			
ksg (year)$^{-1}$	*Ksg* value was calculated by using the chemical half-life in soil, as cited in Howard, Boethling, Jarvis, Meylan, and Michalenko (1991).	B-1-2; B-2-2; B-3-2; B-4-2	5.75E+00
Fv (unitless)	*Fv* value was calculated by using the equation cited in Junge (1977). Recommended	B-1-1; B-2-1;	1.0

TABLE A-3-179

CHEMICAL-SPECIFIC INPUTS FOR 1,1,1,2-TETRACHLOROETHANE (630-20-6)

Parameter	Reference and Explanation	Equations	Value
Biotransfer Factors for Plants			
RCF $(\frac{\mu g/g\ DW\ plant}{\mu g/mL\ soil\ water})$	*RCF* value was calculated by using the correlation equation with K_{ow} that is cited in Briggs (1982). Recommended value was calculated by using the K_{ow} value that is provided in this table. The value was then converted to a dry weight basis by using a moisture content of 87 percent.	B-2-10	3.09E+01
$Br_{rootveg}$ $(\frac{\mu g/g\ DW\ plant}{\mu g/g\ soil})$	$Br_{rootveg}$ value was calculated by dividing the *RCF* value with the Kd_s value provided in this table.	B-2-10	1.94E+01
Br_{ag} $(\frac{\mu g/g\ DW\ plant}{\mu g/g\ soil})$	Br_{ag} value was calculated by using the correlation equation with K_{ow} that is cited in Travis and Arms (1988). No distinction was made between values for aboveground produce and forage. Recommended value was calculated by using the K_{ow} value that is provided in this table.	B-2-9	1.17E+00
Br_{forage} $(\frac{\mu g/g\ DW\ plant}{\mu g/g\ soil})$	Br_{forage} value was calculated by using the correlation equation with K_{ow} that is cited in Travis and Arms (1988). No distinction was made between values for aboveground produce and forage. Recommended value was calculated by using the K_{ow} value that is provided in this table.	B-3-9	1.17E+00
Bv_{ag} $(\frac{\mu g/g\ DW\ plant}{\mu g/g\ air})$	Bv_{ag} value was calculated by using the correlation equation with K_{ow} and *H* that is cited in Bacci, Calamari, Gaggi, and Vighi (1990); and Bacci, Cerejeira, Gaggi, Chemello, Calamari, and Vighi (1992); then reducing this value by a factor of 100. No distinction was made between values for aboveground produce and forage. Recommended value was calculated, for a temperature (T) of 25ºC, by using the *H* and K_{ow} values that are provided in this table.	B-2-8	1.45E-02
Bv_{forage} $(\frac{\mu g/g\ DW\ plant}{\mu g/g\ air})$	Bv_{forage} value was calculated by using the correlation equation with K_{ow} and *H* that is cited in Bacci, Calamari, Gaggi, and Vighi (1990); and Bacci, Cerejeira, Gaggi, Chemello, Calamari, and Vighi (1992); then reducing this value by a factor of 100. No distinction was made between values for aboveground produce and forage. Recommended value was calculated, for a temperature (T) of 25ºC, by using the *H* and K_{ow} values that are provided in this table.	B-3-8	1.45E-02
Biotransfer Factors for Animals			
Ba_{milk} (day/kg FW)	Ba_{milk} value was calculated by using the correlation equation with K_{ow} that is cited in Travis and Arms (1988). Recommended value was calculated by using the K_{ow} value that is provided in this table.	B-3-11	3.39E-06
Ba_{beef} (day/kg FW)	Ba_{beef} value was calculated by using the correlation equation with K_{ow} that is cited in Travis and Arms (1988). Recommended value was calculated by using the K_{ow} value that is provided in this table.	B-3-10	1.07E-05
Ba_{pork} (day/kg FW)	Ba_{pork} value was calculated by using thethe fat content ratio of pork to beef (23/19) and multiplying it with the Ba_{beef} value.	B-3-12	1.30E-05
Ba_{eggs} (day/kg FW)	Ba_{eggs} value was calculated by using the correlation equation with K_{ow} that is cited in California EPA (1993). Recommended value was calculated by using the K_{ow} value that is provided in this table.	B-3-13	3.39E-03
$Ba_{chicken}$ (day/kg FW)	$Ba_{chicken}$ value was calculated by using the fat content ratio of chicken to beef (15/19) and multiplying it with the Ba_{beef} value.	B-3-14	8.46E-06

TABLE A-3-179

CHEMICAL-SPECIFIC INPUTS FOR 1,1,1,2-TETRACHLOROETHANE (630-20-6)

Parameter	Reference and Explanation	Equations	Value
BCF_{fish} (L/kg FW tissue)	*BCFs* were used for compounds with a log K_{ow} value below 4.0, as cited in U.S. EPA (1995b). BCF_{fish} value calculated using the correlation equation with K_{ow} obtained from Veith, Macek, Petrocelli, and Caroll (1980)—See Appendix A-3.	B-4-26	5.87E+01
BAF_{fish} (L/kg FW)	--	B-4-27	NA
$BSAF_{fish}$ (unitless)	--	B-4-28	NA
Health Benchmarks			
RfD (mg/kg/day)	U.S. EPA (1997b)	C-1-8	3.0E-02
Oral CSF $(mg/kg/day)^{-1}$	U.S. EPA (1997b)	C-1-7	2.6E-02
RfC (mg/m^3)	Calculated from *RfD* using an inhalation rate of 20 m^3/day and a human body weight of 70 kg.	C-2-3	1.1E-01
Inhalation URF $(\mu g/m^3)^{-1}$	U.S. EPA (1997b)	C-2-1	7.4E-06
Inhalation CSF $(mg/kg/day)^{-1}$	U.S. EPA (1997c)	C-2-2	2.6E-02

Note:

NA = Not applicable
ND = No data available

All parameters are defined in list of FATE AND TRANSPORT PARAMETERS on page A-3-iii.

TABLE A-3-180

CHEMICAL-SPECIFIC INPUTS FOR 1,1,2,2-TETRACHLOROETHANE (79-34-5)

Parameter	Reference and Explanation	Equations	Value
Chemical/Physical Properties			
MW (g/mole)	Budavari, O'Neil, Smith, and Heckelman (1989)	--	167.86
T_m (K)	Budavari, O'Neil, Smith, and Heckelman (1989)	--	229.1
Vp (atm)	Geometric mean value cited in U.S. EPA (1994c).	--	6.80E-03 at 25°C (liquid)
S (mg/L)	Geometric mean value cited in U.S. EPA (1994c).	--	3.07E+03
H (atm·m^3/mol)	*H* value was calculated by using the theoretical equation from Lyman, Reehl, and Rosenblatt (1982), which defines the constant. Recommended value was calculated by using the *MW*, *S*, and *Vp* values that are provided in this table.	B-1-6; B-2-6; B-2-8; B-3-6; B-4-6; B-4-12; B-4-19	3.72E-04
D_a (cm^2/s)	D_a value was obtained from CHEMDAT8 database (U.S. EPA 1994d).	B-1-6; B-2-6; B-3-6; B-4-6; B-4-21	3.16E-02
D_w (cm^2/s)	D_w value was obtained from CHEMDAT8 database (U.S. EPA 1994d).	B-4-20	9.26E-06
K_{ow} (unitless)	Geometric mean value cited in U.S. EPA (1994c).	--	4.40E+04
K_{oc} (mL/g)	Geometric mean of measured values obtained from U.S. EPA (1996b).	--	7.90E+01
Kd_s (cm^3/g)	Kd_s value was calculated by using the correlation equation with K_{oc} that is cited in U.S. EPA (1993d) for an assumed fraction organic carbon of 0.01 in soil. Measured organic carbon in soil, specific to site conditions, should be used to calculate Kd_s, because the value varies, depending on the fraction of organic carbon in soil. Recommended Kd_s value was calculated by using the K_{oc} value that is provided in this table.	B-1-3; B-1-4; B-1-5; B-1-6; B-2-3; B-2-4; B-2-5; B-2-6; B-2-10; B-3-3; B-3-4; B-3-5; B-3-6; B-4-3; B-4-4; B-4-5; B-4-6; B-4-10; B-4-11	7.90E-01
Kd_{sw} (L/Kg)	Kd_{sw} value was calculated by using the correlation equation with K_{oc} that is cited in U.S. EPA (1993d) for an assumed organic carbon fraction of 0.075 in suspended sediment. Measured organic carbon in suspended sediment, specific to site conditions, should be used to calculate Kd_{sw}, because the value varies, depending on the fraction of organic carbon in suspended sediment. Recommended Kd_{sw} value was calculated by using the K_{oc} value that is provided in this table.	B-4-16; B-4-18; B-4-24	5.93E+00
Kd_{bs} (cm^3/g)	Kd_{bs} value was calculated by using the correlation equation with K_{oc} that is cited in U.S. EPA (1993d) for an assumed organic carbon of 0.04 in bottom sediment. Measured organic carbon in bottom sediment, specific to site conditions, should be used to calculate Kd_{bs}, because the value varies depending on the fraction of organic fraction in bottom sediment. Recommended Kd_{bs} value was calculated by using the K_{oc} value that is provided in this table.	B-4-16; B-4-25	3.16E+00

TABLE A-3-180

CHEMICAL-SPECIFIC INPUTS FOR 1,1,2,2-TETRACHLOROETHANE (79-34-5)

Parameter	Reference and Explanation	Equations	Value
Chemical/Physical Properties (Continued)			
ksg $(year)^{-1}$	*Ksg* value was calculated by using the chemical half-life in soil, as cited in Howard, Boethling, Jarvis, Meylan, and Michalenko (1991).	B-1-2; B-2-2; B-3-2; B-4-2	5.75E+00
Fv (unitless)	*Fv* value was calculated by using the equation cited in Junge (1977). Recommended value of *Fv* was calculated by using the *Vp* value that is provided in this table.	B-1-1; B-2-1; B-2-7; B-2-8; B-3-1; B-3-7; B-3-8; B-4-1; B-4-8; B-4-9; B-4-12; B-5-1	1.0
Biotransfer Factors for Plants			
RCF $(\frac{\mu g/g\ DW\ plant}{\mu g/mL\ soil\ water})$	*RCF* value was calculated by using the correlation equation with K_{ow} that is cited in Briggs (1982). Recommended value was calculated by using the K_{ow} value that is provided in this table. The value was converted to a dry weight basis by using a moisture content of 87 percent.	B-2-10	8.80E+02
$Br_{root\ veg}$ $(\frac{\mu g/g\ DW\ plant}{\mu g/g\ soil})$	$Br_{root\ veg}$ value was calculated by dividing the *RCF* value with the Kd_s value provided in this table (see section A3.4.2 of Appendix A-3).	B-2-10	1.11E+03
Br_{ag} $(\frac{\mu g/g\ DW\ plant}{\mu g/g\ soil})$	Br_{ag} value was calculated by using the correlation equation with K_{ow} that is cited in Travis and Arms (1988). No distinction was made between values for aboveground produce and forage. Recommended value was calculated by using the K_{ow} value that is provided in this table.	B-2-9	8.02E-02
Br_{forage} $(\frac{\mu g/g\ DW\ plant}{\mu g/g\ soil})$	Br_{forage} value was calculated by using the correlation equation with K_{ow} that is cited in Travis and Arms (1988). No distinction was made between values for aboveground produce and forage. Recommended value was calculated by using the K_{ow} value that is provided in this table.	B-3-9	8.02E-02
Bv_{ag} $(\frac{\mu g/g\ DW\ plant}{\mu g/g\ air})$	Bv_{ag} value was calculated by using the correlation equation with K_{ow} and *H* that is cited in Bacci, Calamari, Gaggi, and Vighi (1990); and Bacci, Cerejeira, Gaggi, Chemello, Calamari, and Vighi (1992); then reducing this value by a factor of 100, as recommended by U.S. EPA (1993d). No distinction was made between values for aboveground produce and forage. Recommended value was calculated, for a temperature (T) of 25ºC, by using the *H* and K_{ow} values that are provided in this table.	B-2-8	1.33E+01
Bv_{forage} $(\frac{\mu g/g\ DW\ plant}{\mu g/g\ air})$	Bv_{forage} value was calculated by using the correlation equation with K_{ow} and *H* that is cited in Bacci, Calamari, Gaggi, and Vighi (1990); and Bacci, Cerejeira, Gaggi, Chemello, Calamari, and Vighi (1992); then reducing this value by a factor of 100, as recommended by U.S. EPA (1993d). No distinction was made between values for aboveground produce and forage. Recommended value was calculated, for a temperature (T) of 25ºC, by using the *H* and K_{ow} values that are provided in this table.	B-3-8	1.33E+01
Biotransfer Factors for Animals			
Ba_{milk} (day/kg FW)	Ba_{milk} value was calculated by using the correlation equation with K_{ow} that is cited in Travis and Arms (1988). Recommended value was calculated by using the K_{ow} value that is provided in this table.	B-3-11	3.50E-04

TABLE A-3-180

CHEMICAL-SPECIFIC INPUTS FOR 1,1,2,2-TETRACHLOROETHANE (79-34-5)

Parameter	Reference and Explanation	Equations	Value
Ba_{beef} (day/kg FW)	Ba_{beef} value was calculated by using the correlation equation with K_{ow} that is cited in Travis and Arms (1988). Recommended value was calculated by using the K_{ow} value that is provided in this table.	B-3-10	1.105E-03
Ba_{pork} (day/kg FW)	Ba_{pork} value was calculated by using the fat content ratio of pork to beef (23/19) and multiplying it with the Ba_{beef} value (see section A3.4.2 of Appendix A-3).	B-3-12	1.34E-03
Ba_{egg} (day/kg FW)	Ba_{egg} value was calculated by using the correlation equation with K_{ow} that is cited in California EPA (1993). Recommended value was calculated by using the K_{ow} value that is provided in this table.	B-3-13	3.50E-01
$Ba_{chicken}$ (day/kg FW)	$Ba_{chicken}$ value was calculated by using the fat content ratio of chicken to beef (15/19) and multiplying it with the Ba_{beef} value (see section A3.4.3 of Appendix A-3).	B-3-14	8.73E-04
BCF_{fish} (L/kg FW tissue)	--	B-4-26	NA
BAF_{fish} (L/kg FW)	*BAFs* were used for compounds with a log K_{ow} value above 4.0, as cited in U.S. EPA (1995b). *BAF* values were predicted values calculated by multiplying a food chain multiplier (*FCM*) with a geometric mean of various laboratory measured *BCF*s obtained from various experimental studies cited in U.S. EPA (1998). *FCM*s were obtained from U.S. EPA (1995bc)—See Appendix A-3.	B-4-27	4.33E+03
$BSAF_{fish}$ (unitless)	--	B-4-28	NA
Health Benchmarks			
RfD (mg/kg/day)	--	C-1-8	ND
Oral CSF $(mg/kg/day)^{-1}$	U.S. EPA (1997b)	C-1-7	2.0E-01
RfC (mg/m^3)	--	C-2-3	ND
Inhalation URF $(\mu g/m^3)^{-1}$	U.S. EPA (1997b)	C-2-1	5.8E-05
Inhalation CSF $(mg/kg/day)^{-1}$	U.S. EPA (1997c)	C-2-2	2.0E-01

Note:

NA = Not applicable
ND = No data available

All parameters are defined in list of FATE AND TRANSPORT PARAMETERS on page A-3-iii.

TABLE A-3-181

CHEMICAL-SPECIFIC INPUTS FOR TETRACHLOROETHYLENE (127-18-4)

Parameter	Reference and Explanation	Equations	Value
Chemical/Physical Properties			
MW (g/mole)	Budavari, O'Neil, Smith, and Heckelman (1989)	--	165.85
T_m (K)	Budavari, O'Neil, Smith, and Heckelman (1989)	--	251.1
Vp (atm)	Geometric mean value cited in U.S. EPA (1994c)	--	2.42E-02 at 25°C (liquid)
S (mg/L)	Geometric mean value cited in U.S. EPA (1994c)	--	2.32E+02
H (atm·m^3/mol)	*H* value was calculated by using the theoretical equation from Lyman, Reehl, and Rosenblatt (1982), which defines the constant. Recommended value was calculated by using the *MW*, *S*, and *Vp* values that are provided in this table.	B-1-6; B-2-6; B-2-8; B-3-6; B-4-6; B-4-12; B-4-19	1.73E-02
D_a (cm^2/s)	D_a value was obtained from WATER8 model database (U.S. EPA 1995d).	B-1-6; B-2-6; B-3-6; B-4-6; B-4-21	7.20E-02
D_w (cm^2/s)	D_w value was obtained from WATER8 model database (U.S. EPA 1995d).	B-4-20	8.20E-06
K_{ow} (unitless)	Geometric mean value cited in U.S. EPA (1994c)	--	3.51E+02
K_{oc} (mL/g)	Geometric mean of measured values obtained from U.S. EPA (1996b).	--	2.65E+02
Kd_s (cm^3/g)	Kd_s value was calculated by using the correlation equation with K_{oc} that is cited in U.S. EPA (1993d) for an assumed organic carbon fraction of 0.01 in soil. Measured organic carbon in soil, specific to site conditions, should be used to calculate Kd_s, because the value varies, depending on the fraction of organic carbon in soil. Recommended Kd_s value was calculated by using the K_{oc} value that is provided in this table.	B-1-3; B-1-4; B-1-5; B-1-6; B-2-3; B-2-4; B-2-5; B-2-6; B-2-10; B-3-3; B-3-4; B-3-5; B-3-6; B-4-3; B-4-4; B-4-5; B-4-6; B-4-10; B-4-11	2.65E+00
Kd_{sw} (L/Kg)	Kd_{sw} value was calculated by using the correlation equation with K_{oc} that is cited in U.S. EPA (1993d) for an assumed organic carbon fraction of 0.075 in suspended sediment. Measured organic carbon in suspended sediment, specific to site conditions, should be used to calculate Kd_{sw}, because the value varies, depending on the fraction of organic carbon in suspended sediment. Recommended Kd_{sw} value was calculated by using the K_{oc} value that is provided in this table.	B-4-16; B-4-18; B-4-24	1.99E+01
Kd_{bs} (cm^3/g)	Kd_{bs} value was calculated by using the correlation equation with K_{oc} that is cited in U.S. EPA (1993d) for an assumed organic carbon fraction of 0.04 in bottom sediment. Measured organic carbon in bottom sediment, specific to site conditions, should be used to calculate Kd_{bs}, because the value varies, depending on the fraction of organic carbon in bottom sediment. Recommended Kd_{bs} value was calculated by using the K_{oc} value that is provided in this table.	B-4-16; B-4-25	1.06E+01
Chemical/Physical Properties (Continued)			
ksg (year)$^{-1}$	*ksg* value was calculated by using the chemical half-life in soil, as cited in Howard, Boethling, Jarvis, Meylan, and Michalenko (1991).	B-1-2; B-2-2; B-3-2; B-4-2	7.03E-01
Fv (unitless)	*Fv* value was calculated by using the equation cited in Junge (1977). Recommended value of *Fv* was calculated by using the *Vp* value that is provided in this table.	B-1-1; B-2-1; B-2-7; B-2-8; B-3-1; B-3-7; B-3-8; B-4-1;	1.0

TABLE A-3-181

CHEMICAL-SPECIFIC INPUTS FOR TETRACHLOROETHYLENE (127-18-4)

Parameter	Reference and Explanation	Equations	Value
Biotransfer Factors for Plants			
RCF ($\frac{\mu g/g\ DW\ plant}{\mu g/mL\ soil\ water}$)	*RCF* value was calculated by using the correlation equation with K_{ow} that is cited in Briggs (1982). Recommended value was calculated by using the K_{ow} value that is provided in this table. The value was then converted to a dry weight basis by using a moisture content of 87 percent.	B-2-10	2.75E+01
$Br_{root\ veg}$ ($\frac{\mu g/g\ DW\ plant}{\mu g/g\ soil}$)	$Br_{root\ veg}$ value was calculated by dividing the *RCF* value with the Kd_s value provided in this table.	B-2-10	1.04E-03
Br_{ag} ($\frac{\mu g/g\ DW\ plant}{\mu g/g\ soil}$)	Br_{ag} value was calculated by using the correlation equation with K_{ow} that is cited in Travis and Arms (1988). No distinction was made between values for aboveground produce and forage. Recommended value was calculated by using the K_{ow} value that is provided in this table.	B-2-9	1.31E+00
Br_{forage} ($\frac{\mu g/g\ DW\ plant}{\mu g/g\ soil}$)	Br_{forage} value was calculated by using the correlation equation with K_{ow} that is cited in Travis and Arms (1988). No distinction was made between values for aboveground produce and forage. Recommended value was calculated by using the K_{ow} value that is provided in this table.	B-3-9	1.31E+00
Bv_{ag} ($\frac{\mu g/g\ DW\ plant}{\mu g/g\ air}$)	Bv_{ag} value was calculated by using the correlation equation with K_{ow} and *H* that is cited in Bacci, Calamari, Gaggi, and Vighi (1990); and Bacci, Cerejeira, Gaggi, Chemello, Calamari, and Vighi (1992); then reducing this value by a factor of 100. No distinction was made between values for aboveground produce and forage. Recommended value was calculated, for a temperature (T) of 25ºC, by using the *H* and K_{ow} values that are provided in this table.	B-2-8	1.66E-03
Bv_{forage} ($\frac{\mu g/g\ DW\ plant}{\mu g/g\ air}$)	Bv_{forage} value was calculated by using the correlation equation with K_{ow} and *H* that is cited in Bacci, Calamari, Gaggi, and Vighi (1990); and Bacci, Cerejeira, Gaggi, Chemello, Calamari, and Vighi (1992); then reducing this value by a factor of 100. No distinction was made between values for aboveground produce and forage. Recommended value was calculated, for a temperature (T) of 25ºC, by using the *H* and K_{ow} values that are provided in this table.	B-3-8	1.66E-03
Biotransfer Factors for Animals			
Ba_{milk} (day/kg FW)	Ba_{milk} value was calculated by using the correlation equation with K_{ow} that is cited in Travis and Arms (1988). Recommended value was calculated by using the K_{ow} value that is provided in this table.	B-3-11	2.79E-06
Ba_{beef} (day/kg FW)	Ba_{beef} value was calculated by using the correlation equation with K_{ow} that is cited in Travis and Arms (1988). Recommended value was calculated by using the K_{ow} value that is provided in this table.	B-3-10	8.82E-06
Ba_{pork} (day/kg FW)	Ba_{pork} value was calculated by using the fat content ratio of pork to beef (23/19) and multiplying it with the Ba_{beef} value.	B-3-12	1.07E-05
Ba_{eggs} (day/kg FW)	Ba_{eggs} value was calculated by using the correlation equation with K_{ow} that is cited in California EPA (1993). Recommended value was calculated by using the K_{ow} value that is provided in this table.	B-3-13	2.79E-03
$Ba_{chicken}$ (day/kg FW)	$Ba_{chicken}$ value was calculated by using the fat content ratio of chicken to beef (15/19) and multiplying it with the Ba_{beef} value.	B-3-14	6.96E-06

TABLE A-3-181

CHEMICAL-SPECIFIC INPUTS FOR TETRACHLOROETHYLENE (127-18-4)

Parameter	Reference and Explanation	Equations	Value
BCF_{fish} (L/kg FW tissue)	*BCFs* were used for compounds with a log K_{ow} value below 4.0, as cited in U.S. EPA (1995b). BCF_{fish} value calculated using the correlation equation with K_{ow} obtained from Veith, Macek, Petrocelli, and Caroll (1980)—See Appendix A-3.	B-4-26	5.06E+01
BAF_{fish} (L/kg FW)	--	B-4-27	NA
$BSAF_{fish}$ (unitless)	--	B-4-28	NA
Health Benchmarks			
RfD (mg/kg/day)	U.S. EPA (1997b)	C-1-8	1.0E-02
Oral CSF $(mg/kg/day)^{-1}$	U.S.EPA (1997e)	C-1-7	5.2E-02
RfC (mg/m^3)	Calculated from *RfD* using an inhalation rate of 20 m^3/day and a human body weight of 70 kg.	C-2-3	3.5E-02
Inhalation URF $(\mu g/m^3)^{-1}$	U.S.EPA (1997e)	C-2-1	5.8E-07
Inhalation CSF $(mg/kg/day)^{-1}$	U.S.EPA (1997e)	C-2-2	2.0E-03

Note:

NA= Not applicable
ND= No data available

All parameters are defined in list of FATE AND TRANSPORT PARAMETERS on page A-3-iii.

TABLE A-3-182

CHEMICAL-SPECIFIC INPUTS FOR 2,3,4,6-TETRACHLOROPHENOL (58-90-2)

Parameter	Reference and Explanation	Equations	Value
Chemical/Physical Properties			
MW (g/mole)	U.S. EPA (1995b)	--	231.89
T_m (K)	U.S. EPA (1995b)	--	343.0
Vp (atm)	Geometric mean value cited in U.S. EPA (1994c).	--	6.60E-06 at 25°C (solid)
S (mg/L)	Geometric mean value cited in U.S. EPA (1994c).	--	1.00E+02
H (atm·m^3/mol)	*H* value was calculated by using the theoretical equation from, Lyman, Reehl, and Rosenblatt (1982), which defines the constant. Recommended value was calculated by using the *MW*, *S*, and *Vp* values that are provided in this table.	B-1-6; B-2-6; B-2-8; B-3-6; B-4-6; B-4-12; B-4-19	1.53E-05
D_a (cm^2/s)	D_a value was obtained from WATER8 model database (U.S. EPA 1995d).	B-1-6; B-2-6; B-3-6; B-4-6; B-4-21	2.55E-02
D_w (cm^2/s)	D_w value was obtained from WATER8 model database (U.S. EPA 1995d).	B-4-20	5.78E-06
K_{ow} (unitless)	Geometric mean value cited in U.S. EPA (1994c).	--	2.0E+04
K_{oc} (mL/g)	For all ionizing organics, K_{oc} values were estimated on the basis of pH. Estimated values were obtained from U.S. EPA (1994c).	--	pH / K_{oc} 1 6,190 2 6,188 3 6,166 4 5,956 5 4,456 6 1,323 7 249.2 8 115.3 9 101.6 10 100.2 11 100.0 12 100.0 13 100.0 14 100.0
Kd_s (cm^3/g)	Kd_s value was calculated by using the correlation equation with K_{oc} that is cited in U.S. EPA (1993d) for an assumed fraction organic carbon of 0.01 in soil. Measured organic carbon in soil, specific to site conditions, should be used to calculate Kd_s, because the value varies, depending on the fraction of organic carbon in soil. Recommended Kd_s value was calculated by using the K_{oc} value that is provided in this table for a *pH* of 7.0.	B-1-3; B-1-4; B-1-5; B-1-6; B-2-3; B-2-4; B-2-5; B-2-6; B-2-10; B-3-3; B-3-4; B-3-5; B-3-6; B-4-3; B-4-4; B-4-5; B-4-6; B-4-10; B-4-11	2.49

TABLE A-3-182

CHEMICAL-SPECIFIC INPUTS FOR 2,3,4,6-TETRACHLOROPHENOL (58-90-2)

Parameter	Reference and Explanation	Equations	Value
Chemical/Physical Properties (Continued)			
Kd_{sw} (L/Kg)	Kd_{sw} value was calculated by using the correlation equation with K_{oc} that is cited in U.S. EPA (1993d) for an assumed organic carbon fraction of 0.075 in suspended sediment. Measured organic carbon in suspended sediment, specific to site conditions, should be used to calculate Kd_{sw}, because the value varies, depending on the fraction of organic carbon in suspended sediment. Recommended Kd_{sw} value was calculated by using the K_{oc} value that is provided in this table for a pH of 7.0.	B-4-16; B-4-18; B-4-24	18.69
Kd_{bs} (cm^3/g)	Kd_{bs} value was calculated by using the correlation equation with K_{oc} that is cited in U.S. EPA (1993d) for an assumed organic carbon of 0.04 in bottom sediment. Measured organic carbon in bottom sediment, specific to site conditions, should be used to calculate Kd_{bs}, because the value varies depending on the fraction of organic fraction in bottom sediment. Recommended Kd_{bs} value was calculated by using the K_{oc} value that is provided in this table for a pH of 7.0.	B-4-16; B-4-25	9.97
ksg $(year)^{-1}$	*Ksg* value was calculated by using the chemical half-life in soil, as cited in Howard, Boethling, Jarvis, Meylan, and Michalenko (1991).	B-1-2; B-2-2; B-3-2; B-4-2	1.41
Fv (unitless)	*Fv* value was calculated by using equations cited in Junge (1977) and Bidleman (1988). Recommended value of *Fv* was calculated by using *S*, T_m, and *Vp* values that are provided in this table. *Vp* value for this compound was converted to a liquid-phase value before being used in the calculations.	B-1-1; B-2-1; B-2-7; B-2-8; B-3-1; B-3-7; B-3-8; B-4-1; B-4-8; B-4-9; B-4-12; B-5-1	1.0
Biotransfer Factors for Plants			
RCF $(\frac{\mu g/g\ DW\ plant}{\mu g/mL\ soil\ water})$	*RCF* value was calculated by using the correlation equation with K_{ow} that is cited in Briggs (1982). Recommended value was calculated by using the K_{ow} value that is provided in this table. The value was converted to a dry weight basis by using a moisture content of 87 percent.	B-2-10	4.83E+02
$Br_{root\ veg}$ $(\frac{\mu g/g\ DW\ plant}{\mu g/g\ soil})$	$Br_{root\ veg}$ value was calculated by dividing the *RCF* value with the *Kds* value provided in this table (see section A4.3.2 of Appendix A-3).	B-2-10	1.94E+02
Br_{ag} $(\frac{\mu g/g\ DW\ plant}{\mu g/g\ soil})$	Br_{ag}value was calculated by using the correlation equation with K_{ow} that is cited in Travis and Arms (1988). No distinction was made between values for aboveground produce and forage. Recommended value was calculated by using the K_{ow} value that is provided in this table.	B-2-9	1.27E-01
Br_{forage} $(\frac{\mu g/g\ DW\ plant}{\mu g/g\ soil})$	Br_{forage} value was calculated by using the correlation equation with K_{ow} that is cited in Travis and Arms (1988). No distinction was made between values for aboveground produce and forage. Recommended value was calculated by using the K_{ow} value that is provided in this table.	B-3-9	1.27E-01

TABLE A-3-182

CHEMICAL-SPECIFIC INPUTS FOR 2,3,4,6-TETRACHLOROPHENOL (58-90-2)

Parameter	Reference and Explanation	Equations	Value
Biotransfer Factors for Plants (Continued)			
Bv_{ag} ($\frac{\mu g/g\ DW\ plant}{\mu g/g\ air}$)	Bv_{ag} value was calculated by using the correlation equation with K_{ow} and H that is cited in Bacci, Calamari, Gaggi, and Vighi (1990); and Bacci, Cerejeira, Gaggi, Chemello, Calamari, and Vighi (1992); then reducing this value by a factor of 100, as recommended by U.S. EPA (1993d). No distinction was made between values for aboveground produce and forage. Recommended value was calculated, for a temperature (T) of 25°C, by using the H and K_{ow} values that are provided in this table.	B-3-9	1.39E+02
Bv_{forage} ($\frac{\mu g/g\ DW\ plant}{\mu g/g\ air}$)	Bv_{forage} value was calculated by using the correlation equation with K_{ow} and H that is cited in Bacci, Calamari, Gaggi, and Vighi (1990); and Bacci, Cerejeira, Gaggi, Chemello, Calamari, and Vighi (1992); then reducing this value by a factor of 100, as recommended by U.S. EPA (1993d). No distinction was made between values for aboveground produce and forage. Recommended value was calculated, for a temperature (T) of 25°C, by using the H and K_{ow} values that are provided in this table.	B-3-8	1.39E+02
Biotransfer Factors for Animals			
Ba_{milk} (day/kg FW)	Ba_{milk} value was calculated by using the correlation equation with K_{ow} that is cited in Travis and Arms (1988). Recommended value was calculated by using the K_{ow} value that is provided in this table.	B-3-11	1.59E-04
Ba_{beef} (day/kg FW)	Ba_{beef} value was calculated by using the correlation equation with K_{ow} that is cited in Travis and Arms (1988). Recommended value was calculated by using the K_{ow} value that is provided in this table.	B-3-10	5.02E-04
Ba_{pork} (day/kg FW)	Ba_{pork} value was calculated by using thethe fat content ratio of pork to beef (23/19) and multiplying it with the Ba_{beef} value (see section A4.3.2 of Appendix A-3).	B-3-12	6.08E-04
Ba_{eggs} (day/kg FW)	Ba_{eggs} value was calculated by using the correlation equation with K_{ow} that is cited in California EPA (1993). Recommended value was calculated by using the K_{ow} value that is provided in this table.	B-3-13	1.59E-01
$Ba_{chicken}$ (day/kg FW)	$Ba_{chicken}$ value was calculated by using the fat content ratio of chicken to beef (15/19) and multiplying it with the Ba_{beef} value (see section A4.3.3 of Appendix A-3).	B-3-14	3.97E-04
BCF_{fish} (L/kg, FW tissue)	--	B-4-26	NA
BAF_{fish} (L/kg FW)	*BAF*s were used for compounds with a log K_{ow} value above 4.0, as cited in U.S. EPA (1995b). *BAF* values were predicted values calculated by multiplying a food chain multiplier (*FCM*) with an estimated *BCF*. *BCF*s were estimated using the correlation equation obtained from Veith, Macek, Petrocelli, and Caroll (1980). *FCM*s were obtained from U.S. EPA (1995bc)—See Appendix A-3.	B-4-27	1.63E+03
$BSAF_{fish}$ (unitless)	--	B-4-28	NA

TABLE A-3-182

CHEMICAL-SPECIFIC INPUTS FOR 2,3,4,6-TETRACHLOROPHENOL (58-90-2)

Parameter	Reference and Explanation	Equations	Value
Health Benchmarks			
RfD (mg/kg/day)	U.S. EPA (1997b)	C-1-8	3.0E-02
Oral CSF $(mg/kg/day)^{-1}$	--	C-1-7	ND
RfC (mg/m^3)	Calculated from *RfD* using an inhalation rate of 20 m^3/day and a human body weight of 70 kg.	C-2-3	1.1E-01
Inhalation URF $(\mu g/m^3)^{-1}$	--	C-2-1	ND
Inhalation CSF $(mg/kg/day)^{-1}$	--	C-2-2	ND

Note:

NA = Not applicable
ND = No data available

All parameters are defined in list of FATE AND TRANSPORT PARAMETERS on page A-3-iii.

TABLE A-3-183

CHEMICAL-SPECIFIC INPUTS FOR TETRAHYDROFURAN (109-99-9)

Parameter	Reference and Explanation	Equations	Value
Chemical/Physical Properties			
MW (g/mole)	Montgomery and Welkom (1991)	--	72.1
T_m (K)	Montgomery and Welkom (1991)	--	164.6
Vp (atm)	*Vp* value cited in Budavari, O'Neil, Smith, and Heckleman (1989).	--	2.14E-01 at 25°C (liquid)
S (mg/L)		--	ND
H (atm·m^3/mol)	*H* value was calculated by using the theoretical equation from Lyman, Reehl, and Rosenblatt (1982), which defines the constant. Recommended value was calculated by using the *MW*, *S*, and *Vp* values that are provided in this table.	B-1-6; B-2-6; B-2-8; B-3-6; B-4-6; B-4-12; B-4-19	ND
D_a (cm^2/s)	D_a value was obtained from CHEMDAT8 database (U.S. EPA 1994d).	B-1-6; B-2-6; B-3-6; B-4-6; B-4-21	1.31E-01
D_w (cm^2/s)	D_w value was obtained from CHEMDAT8 database (U.S. EPA 1994d).	B-4-20	1.07E-05
K_{ow} (unitless)	Geometric mean value cited in U.S. EPA (1994g).	--	2.80E+00
K_{oc} (mL/g)	K_{oc} value was calculated by using the correlation equation with K_{ow} for phthalates and PAHs, / all nonionizing organics except phthalates, PAHs, dioxins, and furans, cited in U.S. EPA (1994c). K_{oc} value was calculated by using the recommended K_{ow} value that is provided in this table.	--	3.16E+00
Kd_s (cm^3/g)	Kd_s value was calculated by using the correlation equation with K_{oc} that is cited in U.S. EPA (1993d) for an assumed organic carbon fraction of 0.01 in soil. Measured organic carbon in soil, specific to site conditions, should be used to calculate Kd_s, because the value varies, depending on the fraction of organic carbon in soil. Recommended Kd_s value was calculated by using the K_{oc} value that is provided in this table.	B-1-3; B-1-4; B-1-5; B-1-6; B-2-3; B-2-4; B-2-5; B-2-6; B-2-10; B-3-3; B-3-4; B-3-5; B-3-6; B-4-3; B-4-4; B-4-5; B-4-6; B-4-10; B-4-11	3.16E-02
Kd_{sw} (L/Kg)	Kd_{sw} value was calculated by using the correlation equation with K_{oc} that is cited in U.S. EPA (1993d) for an assumed organic carbon fraction of 0.075 in suspended sediment. Measured organic carbon in suspended sediment, specific to site conditions, should be used to calculate Kd_{sw}, because the value varies, depending on the fraction of organic carbon in suspended sediment. Recommended Kd_{sw} value was calculated by using the K_{oc} value that is provided in this table.	B-4-16; B-4-18; B-4-24	2.37E-01
Chemical/Physical Properties (Continued)			

TABLE A-3-183

CHEMICAL-SPECIFIC INPUTS FOR TETRAHYDROFURAN (109-99-9)

Parameter	Reference and Explanation	Equations	Value
Kd_{bs} (cm^3/g)	Kd_{bs} value was calculated by using the correlation equation with K_{oc} that is cited in U.S. EPA (1993d) for an assumed organic carbon fraction of 0.04 in bottom sediment. Measured organic carbon in bottom sediment, specific to site conditions, should be used to calculate Kd_{bs}, because the value varies, depending on the fraction of organic carbon in bottom sediment. Recommended Kd_{bs} value was calculated by using the K_{oc} value that is provided in this table.	B-4-16; B-4-25	1.26E-01
ksg $(year)^{-1}$	*ksg* value was calculated by using the chemical half-life in soil, as cited in Howard (1989-1993).	B-1-2; B-2-2; B-3-2; B-4-2	4.43E+01
Fv (unitless)	*Fv* value was calculated by using the equation cited in Junge (1977). Recommended value of *Fv* was calculated by using the *Vp* value that is provided in the table.	B-1-1; B-2-1; B-2-7; B-2-8; B-3-1; B-3-7; B-3-8; B-4-1; B-4-8; B-4-9; B-4-12; B-5-1	1.00
Biotransfer Factors for Plants			
RCF $(\frac{\mu g/g\ DW\ plant}{\mu g/mL\ soil\ water})$	*RCF* value was calculated by using the correlation equation with K_{ow} that is cited in Briggs (1982). Recommended value was calculated by using the K_{ow} value that is provided in this table. The value was then converted to a dry weight basis by using a moisture content of 87 percent.	B-2-10	6.82E+00
$Br_{root\ veg}$ $(\frac{\mu g/g\ DW\ plant}{\mu g/g\ soil})$	$Br_{root\ veg}$ value was calculated by dividing the *RCF* value with the Kd_s value provided in this table.	B-2-10	2.16E+02
Br_{ag} $(\frac{\mu g/g\ DW\ plant}{\mu g/g\ soil})$	Br_{ag} value was calculated by using the correlation equation with K_{ow} that is cited in Travis and Arms (1988). No distinction was made between values for aboveground produce and forage. Recommended value was calculated by using the K_{ow} value that is provided in this table.	B-2-9	2.14E+01
Br_{forage} $(\frac{\mu g/g\ DW\ plant}{\mu g/g\ soil})$	Br_{forage} value was calculated by using the correlation equation with K_{ow} that is cited in Travis and Arms (1988). No distinction was made between values for abovegroud produce and forage. Recommended value was calculated by using the K_{ow} value that is provided in this table.	B-3-9	2.14E+01
Bv_{ag} $(\frac{\mu g/g\ DW\ plant}{\mu g/g\ air})$		B-2-8	ND
Bv_{forage} $(\frac{\mu g/g\ DW\ plant}{\mu g/g\ air})$		B-3-8	ND
Biotransfer Factors for Animals			
Ba_{milk} (day/kg FW)	Ba_{milk} value was calculated by using the correlation equation with K_{ow} that is cited in Travis and Arms (1988). Recommended value was calculated by using the K_{ow} value that is provided in this table.	B-3-11	2.22E-08

TABLE A-3-183

CHEMICAL-SPECIFIC INPUTS FOR TETRAHYDROFURAN (109-99-9)

Parameter	Reference and Explanation	Equations	Value
Ba_{beef} (day/kg FW)	Ba_{beef} value was calculated by using the correlation equation with K_{ow} that is cited in Travis and Arms (1988). Recommended value was calculated by using the K_{ow} value that is provided in this table.	B-3-10	7.03E-08
Ba_{pork} (day/kg FW)	Ba_{pork} value was calculated by using the fat content ratio of pork to beef (23/19) and multiplying it with the Ba_{beef} value.	B-3-12	8.51E-08
Ba_{egg} (day/kg FW)	Ba_{egg} value was calculated by using the correlation equation with K_{ow} that is cited in California EPA (1993). Recommended value was calculated by using the K_{ow} value that is provided in this table.	B-3-13	2.22E-05
$Ba_{chicken}$ (day/kg FW)	$Ba_{chicken}$ value was calculated by using the fat content ratio of chicken to beef (15/19) and multiplying it with the Ba_{beef} value.	B-3-14	5.55E-08
BCF_{fish} (L/kg FW tissue)	*BCFs* were used for compounds with a log K_{ow} value below 4.0, as cited in U.S. EPA (1995b). BCF_{fish} value calculated using the correlation equation with K_{ow} obtained from Veith, Macek, Petrocelli, and Caroll (1980)—See Appendix A-3.	B-4-26	1.29E+00
BAF_{fish} (L/kg FW)	--	B-4-27	NA
$BSAF_{fish}$ (unitless)	--	B-4-28	NA
Health Benchmarks			
RfD (mg/kg/day)	--	C-1-8	ND
Oral CSF $(mg/kg/day)^{-1}$	--	C-1-7	ND
RfC (mg/m^3)	--	C-2-3	ND
Inhalation URF $(\mu g/m^3)^{-1}$	--	C-2-1	ND
Inhalation CSF $(mg/kg/day)^{-1}$	--	C-2-2	ND

Note:

NA = Not applicable
ND = No data available

All parameters are defined in list of FATE AND TRANSPORT PARAMETERS on page A-3-iii.

TABLE A-3-184

CHEMICAL-SPECIFIC INPUTS FOR THALLIUM (7440-28-0)

Parameter	Reference and Explanation	Equations	Value
Chemical/Physical Properties			
MW (g/mole)	Budavari, O'Neil, Smith, and Heckelman (1989)	--	204.38
T_m (^{o}K)	Budavari, O'Neil, Smith, and Heckelman (1989)	--	576.6
Vp (atm)	All metals, except mercury, are assumed to be nonvolatile at ambient temperatures.	--	0.0
S (mg/L)	All metals, except mercury, are assumed to be insoluble in water.	--	0.0
H (atm·m^3/mol)	*H* value is assumed to be zero, because the *Vp* and *S* values are zero for all metals, except mercury.	B-1-6; B-2-6; B-2-8; B-3-6; B-4-6; B-4-12; B-4-19	0.0
D_a (cm^2/s)	D_a value was calculated using the equation cited in U.S. EPA (1996a).	B-1-6; B-2-6; B-3-6; B-4-6; B-4-21	5.48E-02
D_w (cm^2/s)	D_w value was calculated using the equation cited in U.S. EPA (1996a).	B-4-20	6.34E-06
K_{ow} (unitless)	--	--	NA
K_{oc} (mL/g)	--	--	NA
Kd_s (mL/g)	Kd_s value was obtained from U.S. EPA (1996a), which provides pH-based values that were estimated by using the MINTEQ2 geochemical speciation model.	B-1-3; B-1-4; B-1-5; B-1-6; B-2-3; B-2-4; B-2-5; B-2-6; B-2-10; B-3-3; B-3-4; B-3-5; B-3-6; B-4-3; B-4-4; B-4-5; B-4-6; B-4-10; B-4-11	44 at pH=4.9; 71 at pH=6.8; 96 at pH=8.0
Kd_{sw} (L/Kg)	Kd_{sw} value is assumed to be same as the Kd_s value, because organic carbon does not play a major role in sorption for the metals, as cited in U.S. EPA (1994f).	B-4-16; B-4-18; B-4-24	44 at pH=4.9; 71 at pH=6.8; 96 at pH=8.0
Kd_{bs} (mL/g)	Kd_{bs} value is assumed to be same as the Kd_s value, because organic carbon does not play a major role in sorption for the metals, as cited in U.S. EPA (1994f).	B-4-16; B-4-25	44 at pH=4.9; 71 at pH=6.8; 96 at pH=8.0
ksg (year)$^{-1}$	--	B-1-2; B-2-2; B-3-2; B-4-2	ND

TABLE A-3-184

CHEMICAL-SPECIFIC INPUTS FOR THALLIUM (7440-28-0)

Parameter	Reference and Explanation	Equations	Value
Chemical/Physical Properties (Continued)			
Fv (unitless)	Because they are nonvolatile, metals are assumed to be 100 percent in particulate phase and zero percent in the vapor phase, as cited in U.S. EPA (1994f).	B-1-1; B-2-1; B-2-7; B-2-8; B-3-1; B-3-7; B-3-8; B-4-1; B-4-8; B-4-9; B-4-12; B-5-1	0.0
Biotransfer Factors for Plants			
RCF $(\frac{\mu g/g\ DW\ plant}{\mu g/mL\ soil\ water})$	--	B-2-10	ND
$Br_{rootveg}$ $(\frac{\mu g/g\ DW\ plant}{\mu g/g\ soil})$	$Br_{rootveg}$ value was obtained from Baes, Sharp, Sjoreen, and Shor (1984). *Br* values for nonvegetative growth (such as tubers) in Baes, Sharp, Sjoreen, and Shor (1984) were used for $Br_{root\ veg}$.	B-2-10	4.00E-04
Br_{ag} $(\frac{\mu g/g\ DW\ plant}{\mu g/g\ soil})$	Br_{ag} value for fruits was obtained from Baes, Sharp, Sjoreen, and Shor (1984). *Br* values for nonvegetative growth (reproductive) in Baes, Sharp, Sjoreen, and Shor (1984) were used for Br_{ag} (fruits). Br_{ag} value for vegetables was calculated using data obtained from Baes, Sharp, Sjoreen, and Shor (1984). *Br* values for nonvegetative (reproductive) growth and *Bv* values for vegetative growth weighted as 75% (reproductive) and 25% vegetative (Baes, Sharp, Sjoreen, and Shor [1984])—were used for Br_{ag} (vegetables). The weighted average Br_{ag} value for aboveground produce was obtained as follows: (1) Br_{ag} values for fruits combined with a human consumption rate of fruits of 1.44E-03 kg/kg/day, and (2) Br_{ag} values for vegetables combined with a human consumption rate of vegetables of 1.49E-03 kg/kg/day.	B-2-9	8.58E-04
Br_{forage} $(\frac{\mu g/g\ DW\ plant}{\mu g/g\ soil})$	Br_{forage} value was obtained from Baes, Sharp, Sjoreen, and Shor (1984). *Bv* values for vegetative growth (such as leaves and stems) in Baes, Sharp, Sjoreen, and Shor (1984) were used for Br_{forage}.	B-3-8	4.00E-03
Br_{grain} $(\frac{\mu g/g\ DW\ plant}{\mu g/g\ soil})$	Br_{grain} value was obtained from Baes, Sharp, Sjoreen, and Shor (1984). *Br* values for nonvegetative growth as recommended by Baes, Sharp, Sjoreen, and Shor (1984) were used for Br_{grain}.	B-3-8	4.00E-04
Bv_{ag} $(\frac{\mu g/g\ DW\ plant}{\mu g/g\ air})$	Metals are assumed to not experience air-to-leaf transfer, as cited in U.S. EPA (1995b).	B-2-8	NA
Bv_{forage} $(\frac{\mu g/g\ DW\ plant}{\mu g/g\ air})$	Metals are assumed to not experience air-to-leaf transfer, as cited in U.S. EPA (1995b).	B-3-8	NA

TABLE A-3-184

CHEMICAL-SPECIFIC INPUTS FOR THALLIUM (7440-28-0)

Parameter	Reference and Explanation	Equations	Value
Biotransfer Factors for Animals			
Ba_{milk} (day/kg FW)	Ba_{milk} values were obtained from Baes, Sharp, Sjoreen, and Shor (1984) for all metals, except cadmium, mercury, selenium, and zinc.	B-3-11	2.0E-03
Ba_{beef} (day/kg FW)	Ba_{beef} values were obtained from Baes, Sharp, Sjoreen, and Shor (1984) for all metals, except cadmium, mercury, selenium, and zinc.	B-3-10	4.0E-02
Ba_{pork} (day/kg FW)	--	B-3-12	ND
Ba_{eggs} (day/kg FW)	--	B-3-13	ND
$Ba_{chicken}$ (day/kg FW)	--	B-3-14	ND
BCF_{fish} (L/kg FW tissue)	Geometric mean value obtained from various literature sources (see Appendix A3.4).	B-4-26	1.40E+03
BAF_{fish} (L/kg FW)	--	B-4-27	NA
$BSAF_{fish}$ (unitless)	--	B-4-28	NA
Health Benchmarks			
RfD (mg/kg/day)	U.S. EPA (1997b)	C-1-8	8.0E-05
Oral CSF $(mg/kg/day)^{-1}$	--	C-1-7	ND
RfC (mg/m^3)	Calculated from *RfD* using an inhalation rate of 20 m^3/day and a human body weight of 70 kg.	C-2-3	2.8E-04
Inhalation URF $(\mu g/m^3)^{-1}$	--	C-2-1	ND
Inhalation CSF $(mg/kg/day)^{-1}$	--	C-2-2	ND

Note:

All parameters are defined in list of FATE AND TRANSPORT PARAMETERS on page A-3-iii.

TABLE A-3-185

CHEMICAL-SPECIFIC INPUTS FOR TOLUENE (108-88-3)

Parameter	Reference and Explanation	Equations	Value
Chemical/Physical Properties			
MW (g/mole)	Budavari, O'Neil, Smith, and Heckelman (1989)	--	92.13
T_m (K)	Budavari, O'Neil, Smith, and Heckelman (1989)	--	178.1
Vp (atm)	Geometric mean value cited in U.S. EPA (1994c)	--	3.71E-02 at 25°C (liquid)
S (mg/L)	Geometric mean value cited in U.S. EPA (1994c)	--	5.58E+02
H (atm·m^3/mol)	*H* value was calculated by using the theoretical equation from Lyman, Reehl, and Rosenblatt (1982), which defines the constant. Recommended value was calculated by using the *MW*, *S*, and *Vp* values that are provided in this table.	B-1-6; B-2-6; B-2-8; B-3-6; B-4-6; B-4-12; B-4-19	6.13E-03
D_a (cm^2/s)	D_a value was obtained from CHEMDAT8 database (U.S. EPA 1994d).	B-1-6; B-2-6; B-3-6; B-4-6; B-4-21	9.72E-02
D_w (cm^2/s)	D_w value was obtained from CHEMDAT8 database (U.S. EPA 1994d).	B-4-20	9.23E-06
K_{ow} (unitless)	Geometric mean value cited in U.S. EPA (1994c)	--	4.65E+02
K_{oc} (mL/g)	Geometric mean of measured values obtained from U.S. EPA (1996b).	--	1.40E+02
Kd_s (cm^3/g)	Kd_s value was calculated by using the correlation equation with K_{oc} that is cited in U.S. EPA (1993d) for an assumed organic carbon fraction of 0.01 in soil. Measured organic carbon in soil, specific to site conditions, should be used to calculate Kd_s, because the value varies, depending on the fraction of organic carbon in soil. Recommended Kd_s value was calculated by using the K_{oc} value that is provided in this table.	B-1-3; B-1-4; B-1-5; B-1-6; B-2-3; B-2-4; B-2-5; B-2-6; B-2-10; B-3-3; B-3-4; B-3-5; B-3-6; B-4-3; B-4-4; B-4-5; B-4-6; B-4-10; B-4-11	1.40E+00
Kd_{sw} (L/Kg)	Kd_{sw} value was calculated by using the correlation equation with K_{oc} that is cited in U.S. EPA (1993d) for an assumed organic carbon fraction of 0.075 in suspended sediment. Measured organic carbon in suspended sediment, specific to site conditions, should be used to calculate Kd_{sw}, because the value varies, depending on the fraction of organic carbon in suspended sediment. Recommended Kd_{sw} value was calculated by using the K_{oc} value that is provided in this table.	B-4-16; B-4-18; B-4-24	1.05E+01
Kd_{bs} (cm^3/g)	Kd_{bs} value was calculated by using the correlation equation with K_{oc} that is cited in U.S. EPA (1993d) for an assumed organic carbon fraction of 0.04 in bottom sediment. Measured organic carbon in bottom sediment, specific to site conditions, should be used to calculate Kd_{bs}, because the value varies, depending on the fraction of organic carbon in bottom sediment. Recommended Kd_{bs} value was calculated by using the K_{oc} value that is provided in this table.	B-4-16; B-4-25	5.60E+00
Chemical/Physical Properties (Continued)			
ksg (year)$^{-1}$	*ksg* value was calculated by using the chemical half-life in soil, as cited in Howard, Boethling, Jarvis, Meylan, and Michalenko (1991) and Mackay, Shiu, and Ma (1992).	B-1-2; B-2-2; B-3-2; B-4-2	1.15E+01
Fv (unitless)	*Fv* value was calculated by using the equation cited in Junge (1977). Recommended value of *Fv* was calculated by using the *Vp* value that is provided in this table.	B-1-1; B-2-1; B-2-7; B-2-8; B-3-1; B-3-7;	1.0

TABLE A-3-185

CHEMICAL-SPECIFIC INPUTS FOR TOLUENE (108-88-3)

Parameter	Reference and Explanation	Equations	Value
Biotransfer Factors for Plants			
RCF $(\frac{\mu g/g\ DW\ plant}{\mu g/mL\ soil\ water})$	RCF value was calculated by using the correlation equation with K_{ow} that is cited in Briggs (1982). Recommended value was calculated by using the K_{ow} value that is provided in this table. The value was then converted to a dry weight basis by using a moisture content of 87 percent.	B-2-10	3.26E+01
$Br_{root\ veg}$ $(\frac{\mu g/g\ DW\ plant}{\mu g/g\ soil})$	$Br_{root\ veg}$ value was calculated by dividing the RCF value with the Kd_s value provided in this table.	B-2-10	2.33E+01
Br_{ag} $(\frac{\mu g/g\ DW\ plant}{\mu g/g\ soil})$	Br_{ag} value was calculated by using the correlation equation with K_{ow} that is cited in Travis and Arms (1988). No distinction was made between values for aboveground produce and forage. Recommended value was calculated by using the K_{ow} value that is provided in this table.	B-2-9	1.11E+00
Br_{forage} $(\frac{\mu g/g\ DW\ plant}{\mu g/g\ soil})$	Br_{forage} value was calculated by using the correlation equation with K_{ow} that is cited in Travis and Arms (1988). No distinction was made between values for abovegroud produce and forage. Recommended value was calculated by using the K_{ow} value that is provided in this table.	B-3-9	1.11E+00
Bv_{ag} $(\frac{\mu g/g\ DW\ plant}{\mu g/g\ air})$	Bv_{ag} value was calculated by using the correlation equation with K_{ow} and H that is cited in Bacci, Calamari, Gaggi, and Vighi (1990); and Bacci, Cerejeira, Gaggi, Chemello, Calamari, and Vighi (1992); then reducing this value by a factor of 100. No distinction was made between values for aboveground produce and forage. Recommended value was calculated, for a temperature (T) of 25ºC, by using the H and K_{ow} values that are provided in this table.	B-2-8	6.33E-03
Bv_{forage} $(\frac{\mu g/g\ DW\ plant}{\mu g/g\ air})$	Bv_{forage} value was calculated by using the correlation equation with K_{ow} and H that is cited in Bacci, Calamari, Gaggi, and Vighi (1990); and Bacci, Cerejeira, Gaggi, Chemello, Calamari, and Vighi (1992); then reducing this value by a factor of 100. No distinction was made between values for aboveground produce and forage. Recommended value was calculated, for a temperature (T) of 25ºC, by using the H and K_{ow} values that are provided in this table.	B-3-8	6.33E-03
Biotransfer Factors for Animals			
Ba_{milk} (day/kg FW)	Ba_{milk} value was calculated by using the correlation equation with K_{ow} that is cited in Travis and Arms (1988). Recommended value was calculated by using the K_{ow} value that is provided in this table.	B-3-11	3.69E-06
Ba_{beef} (day/kg FW)	Ba_{beef} value was calculated by using the correlation equation with K_{ow} that is cited in Travis and Arms (1988). Recommended value was calculated by using the K_{ow} value that is provided in this table.	B-3-10	1.17E-05
Ba_{pork} (day/kg FW)	Ba_{pork} value was calculated by using the fat content ratio of pork to beef (23/19) and multiplying it with the Ba_{beef} value.	B-3-12	1.41E-05
Ba_{eggs} (day/kg FW)	Ba_{eggs} value was calculated by using the correlation equation with K_{ow} that is cited in California EPA (1993). Recommended value was calculated by using the K_{ow} value that is provided in this table.	B-3-13	3.69E-03
$Ba_{chicken}$ (day/kg FW)	$Ba_{chicken}$ value was calculated by using the fat content ratio of chicken to beef (15/19) and multiplying it with the Ba_{beef} value.	B-3-14	9.22E-06

TABLE A-3-185

CHEMICAL-SPECIFIC INPUTS FOR TOLUENE (108-88-3)

Parameter	Reference and Explanation	Equations	Value
BCF_{fish} (L/kg FW tissue)	*BCFs* were used for compounds with a log K_{ow} value below 4.0, as cited in U.S. EPA (1995b). BCF_{fish} value calculated using the correlation equation with K_{ow} obtained from Veith, Macek, Petrocelli, and Caroll (1980)—See Appendix A-3.	B-4-26	6.27E+01
BAF_{fish} (L/kg FW)	--	B-4-27	NA
$BSAF_{fish}$ (unitless)	--	B-4-28	NA
Health Benchmarks			
RfD (mg/kg/day)	U.S. EPA (1997b)	C-1-8	2.0E-01
Oral CSF $(mg/kg/day)^{-1}$	--	C-1-7	ND
RfC (mg/m^3)	U.S. EPA (1997b)	C-2-3	4.0E-01
Inhalation URF $(\mu g/m^3)^{-1}$	--	C-2-1	ND
Inhalation CSF $(mg/kg/day)^{-1}$	--	C-2-2	ND

Note:

NA= Not applicable
ND= No data available

All parameters are defined in list of FATE AND TRANSPORT PARAMETERS on page A-3-iii.

TABLE A-3-186

CHEMICAL-SPECIFIC INPUTS FOR O-TOLUIDINE (95-53-4)

Parameter	Reference and Explanation	Equations	Value
Chemical/Physical Properties			
MW (g/mole)	Budavari, O'Neill, Smith, and Heckelman (1989)	--	107.15
T_m (K)	Montgomery and Welkom (1991)	--	258.4
Vp (atm)	*Vp* value cited in U.S. EPA (1995b).	--	3.94E-04 at 25°C (liquid)
S (mg/L)	*S* value cited in U.S. EPA (1995b).	--	1.74E+04
H (atm·m^3/mol)	*H* value was calculated by using the theoretical equation from Lyman, Reehl, and Rosenblatt (1982), which defines the constant. Recommended value was calculated by using the *MW*, *S*, and *Vp* values that are provided in this table.	B-1-6; B-2-6; B-2-8; B-3-6; B-4-6; B-4-12; B-4-19	2.43E-06
D_a (cm^2/s)	D_a value was obtained from CHEMDAT8 database (U.S. EPA 1994d).	B-1-6; B-2-6; B-3-6; B-4-6; B-4-21	7.14E-02
D_w (cm^2/s)	D_w value was obtained from CHEMDAT8 database (U.S. EPA 1994d).	B-4-20	9.12E-06
K_{ow} (unitless)	Arithmetic mean value cited in Karickhoff and Long (1995).	--	2.19E+01
K_{oc} (mL/g)	K_{oc} value was calculated by using the correlation equation with K_{ow} for all nonionizing organics except phthalates, PAHs, dioxins, and furans as cited in U.S. EPA (1994c). K_{oc} value was calculated by using the recommended K_{ow} value that is provided in this table.	--	1.57E+01
Kd_s (cm^3/g)	Kd_s value was calculated by using the correlation equation with K_{oc} that is cited in U.S. EPA (1993d) for an assumed fraction organic carbon of 0.01 in soil. Measured organic carbon in soil, specific to site conditions, should be used to calculate Kd_s, because the value varies, depending on the fraction of organic carbon in soil. Recommended Kd_s value was calculated by using the K_{oc} value that is provided in this table.	B-1-3; B-1-4; B-1-5; B-1-6; B-2-3; B-2-4; B-2-5; B-2-6; B-2-10; B-3-3; B-3-4; B-3-5; B-3-6; B-4-3; B-4-4; B-4-5; B-4-6; B-4-10; B-4-11	1.57E-01
Kd_{sw} (L/Kg)	Kd_{sw} value was calculated by using the correlation equation with K_{oc} that is cited in U.S. EPA (1993d) for an assumed organic carbon fraction of 0.075 in suspended sediment. Measured organic carbon in suspended sediment, specific to site conditions, should be used to calculate Kd_{sw}, because the value varies, depending on the fraction of organic carbon in suspended sediment. Recommended Kd_{sw} value was calculated by using the K_{oc} value that is provided in this table.	B-4-16; B-4-18; B-4-24	1.18E+00
Kd_{bs} (cm^3/g)	Kd_{bs} value was calculated by using the correlation equation with K_{oc} that is cited in U.S. EPA (1993d) for an assumed organic carbon of 0.04 in bottom sediment. Measured organic carbon in bottom sediment, specific to site conditions, should be used to calculate Kd_{bs}, because the value varies depending on the fraction of organic fraction in bottom sediment. Recommended Kd_{bs} value was calculated by using the K_{oc} value that is provided in this table.	B-4-16; B-4-25	6.28E-01

TABLE A-3-186

CHEMICAL-SPECIFIC INPUTS FOR O-TOLUIDINE (95-53-4)

Parameter	Reference and Explanation	Equations	Value
Chemical/Physical Properties (Continued)			
ksg $(year)^{-1}$	*ksg* value was calculated by using the chemical half-life in soil, as cited in Howard, Boethling, Jarvis, Meylan, and Michalenko (1991).	B-1-2; B-2-2; B-3-2; B-4-2	3.61E+01
Fv (unitless)	*Fv* value was calculated by using the equation cited in Junge (1977). Recommended value of *Fv* was calculated by using the *Vp* value that is provided in this table.	B-1-1; B-2-1; B-2-7; B-2-8; B-3-1; B-3-7; B-3-8; B-4-1; B-4-8; B-4-9; B-4-12; B-5-1	1.0
Biotransfer Factors for Plants			
RCF $(\frac{\mu g/g\ DW\ plant}{\mu g/mL\ soil\ water})$	*RCF* value was calculated by using the correlation equation with K_{ow} that is cited in Briggs (1982). Recommended value was calculated by using the K_{ow} value that is provided in this table. The value was converted to a dry weight basis by using a moisture content of 87 percent.	B-2-10	8.81E+00
$Br_{root\ veg}$ $(\frac{\mu g/g\ DW\ plant}{\mu g/g\ soil})$	$Br_{root\ veg}$ value was calculated by dividing the *RCF* value with the Kd_s value provided in this table.	B-2-10	5.61E+01
Br_{ag} $(\frac{\mu g/g\ DW\ plant}{\mu g/g\ soil})$	Br_{ag} value was calculated by using the correlation equation with K_{ow} that is cited in Travis and Arms (1988). No distinction was made between values for aboveground produce and forage. Recommended value was calculated by using the K_{ow} value that is provided in this table.	B-2-9	6.51E+00
Br_{forage} $(\frac{\mu g/g\ DW\ plant}{\mu g/g\ soil})$	Br_{forage} value was calculated by using the correlation equation with K_{ow} that is cited in Travis and Arms (1988). No distinction was made between values for aboveground produce and forage. Recommended value was calculated by using the K_{ow} value that is provided in this table.	B-3-9	6.51E+00
Bv_{ag} $(\frac{\mu g/g\ DW\ plant}{\mu g/g\ air})$	Bv_{ag} value was calculated by using the correlation equation with K_{ow} and *H* that is cited in Bacci, Calamari, Gaggi, and Vighi (1990); and Bacci, Cerejeira, Gaggi, Chemello, Calamari, and Vighi (1992); then reducing this value by a factor of 100, as recommended by U.S. EPA (1993d). No distinction was made between values for aboveground produce and forage. Recommended value was calculated, for a temperature (T) of 25°C, by using the *H* and K_{ow} values that are provided in this table.	B-2-8	6.16E-01
Bv_{forage} $(\frac{\mu g/g\ DW\ plant}{\mu g/g\ air})$	Bv_{forage} value was calculated by using the correlation equation with K_{ow} and *H* that is cited in Bacci, Calamari, Gaggi, and Vighi (1990); and Bacci, Cerejeira, Gaggi, Chemello, Calamari, and Vighi (1992); then reducing this value by a factor of 100, as recommended by U.S. EPA (1993d). No distinction was made between values for aboveground produce and forage. Recommended value was calculated, for a temperature (T) of 25°C, by using the *H* and K_{ow} values that are provided in this table.	B-3-8	6.16E-01
Biotransfer Factors for Animals			
Ba_{milk} (day/kg FW)	Ba_{milk} value was calculated by using the correlation equation with K_{ow} that is cited in Travis and Arms (1988). Recommended value was calculated by using the K_{ow} value that is provided in this table.	B-3-11	1.74E-07

TABLE A-3-186

CHEMICAL-SPECIFIC INPUTS FOR O-TOLUIDINE (95-53-4)

Parameter	Reference and Explanation	Equations	Value
Ba_{beef} (day/kg FW)	Ba_{beef} value was calculated by using the correlation equation with K_{ow} that is cited in Travis and Arms (1988). Recommended value was calculated by using the K_{ow} value that is provided in this table.	B-3-10	5.50E-07
Ba_{pork} (day/kg FW)	Ba_{pork} value was calculated by using the fat content ratio of pork to beef (23/19) and multiplying it with the Ba_{beef} value.	B-3-12	6.65E-07
Ba_{eggs} (day/kg FW)	Ba_{eggs} value was calculated by using the correlation equation with K_{ow} that is cited in California EPA (1993). Recommended value was calculated by using the K_{ow} value that is provided in this table.	B-3-13	1.74E-04
$Ba_{chicken}$ (day/kg FW)	$Ba_{chicken}$ value was calculated by using the fat content ratio of chicken to beef (15/19) and multiplying it with the Ba_{beef} value.	B-3-14	4.34E-07
BCF_{fish} (L/kg, FW tissue)	*BCFs* were used for compounds with a log K_{ow} value below 4.0, as cited in U.S. EPA (1995b). BCF_{fish} value calculated using the correlation equation with K_{ow} obtained from Veith, Macek, Petrocelli, and Caroll (1980)—See Appendix A-3.	B-4-26	6.14E+00
BAF_{fish} (L/kg FW)	--	B-4-27	NA
$BSAF_{fish}$ (unitless)	--	B-4-28	NA
Health Benchmarks			
RfD (mg/kg/day)	--	C-1-8	NA
Oral CSF $(mg/kg/day)^{-1}$	U.S. EPA (1995b)	C-1-7	2.4E-01
RfC (mg/m^3)	--	C-2-3	NA
Inhalation URF $(\mu g/m^3)^{-1}$	Calculated from *Oral CSF* using an inhalation rate of 20 m^3/day and a human body weight of 70 kg.	C-2-1	6.9E-02
Inhalation CSF $(mg/kg/day)^{-1}$	Value beased on Oral CSF assuming route-to-route extrapolation.	C-2-2	2.4E-01

Note:

NA= Not applicable
ND= No data available

All parameters are defined in list of FATE AND TRANSPORT PARAMETERS on page A-3-iii.

TABLE A-3-187

CHEMICAL-SPECIFIC INPUTS FOR 1,2,3-TRICHLOROBENZENE (87-61-6)

Parameter	Reference and Explanation	Equations	Value
Chemical/Physical Properties			
MW (g/mole)	Budavari, O'Neil, Smith, and Heckelman (1989)	--	181.46
T_m (K)	Budavari, O'Neil, Smith, and Heckelman (1989)	--	325.7
Vp (atm)	Geometric mean value calculated from values cited in Mackay, Shiu, and Ma (1991).	--	3.20E-04 at 25°C (solid)
S (mg/L)	Geometric mean value calculated from values cited in Mackay, Shiu, and Ma (1991).	--	2.05E+01
H (atm·m^3/mol)	*H* value was calculated by using the theoretical equation from Lyman, Reehl, and Rosenblatt (1982), which defines the constant. Recommended value was calculated by using the *MW*, *S*, and *Vp* values that are provided in this table.	B-1-6; B-2-6; B-2-8; B-3-6; B-4-6; B-4-12; B-4-19	2.84E-03
D_a (cm^2/s)	D_a value was obtained from CHEMDAT8 database (U.S. EPA 1994d).	B-1-6; B-2-6; B-3-6; B-4-6; B-4-21	3.02E-02
D_w (cm^2/s)	D_w value was obtained from CHEMDAT8 database (U.S. EPA 1994d).	B-4-20	8.15E-06
K_{ow} (unitless)	Arithmetic mean value cited in Karickhoff and Long (1995).	--	1.11E+04
K_{oc} (mL/g)	K_{oc} value was calculated by using the correlation equation with K_{ow} for phthalates and PAHs, / all nonionizing organics except phthalates, PAHs, dioxins, and furans, cited in U.S. EPA (1994c). K_{oc} value was calculated by using the recommended K_{ow} value that is provided in this table.	--	2.02E+04
Kd_s (cm^3/g)	Kd_s value was calculated by using the correlation equation with K_{oc} that is cited in U.S. EPA (1993d) for an assumed organic carbon fraction of 0.01 in soil. Measured organic carbon in soil, specific to site conditions, should be used to calculate Kd_s, because the value varies, depending on the fraction of organic carbon in soil. Recommended Kd_s value was calculated by using the K_{oc} value that is provided in this table.	B-1-3; B-1-4; B-1-5; B-1-6; B-2-3; B-2-4; B-2-5; B-2-6; B-3-3; B-3-4; B-3-5; B-3-6; B-4-3; B-4-4; B-4-5; B-4-6; B-4-10; B-4-11	2.02E+02
Kd_{sw} (L/Kg)	Kd_{sw} value was calculated by using the correlation equation with K_{oc} that is cited in U.S. EPA (1993d) for an assumed organic carbon fraction of 0.075 in suspended sediment. Measured organic carbon in suspended sediment, specific to site conditions, should be used to calculate Kd_{sw}, because the value varies, depending on the fraction of organic carbon in suspended sediment. Recommended Kd_{sw} value was calculated by using the K_{oc} value that is provided in this table.	B-4-16; B-4-18; B-4-24	1.52E+03
Kd_{bs} (cm^3/g)	Kd_{bs} value was calculated by using the correlation equation with K_{oc} that is cited in U.S. EPA (1993d) for an assumed organic carbon fraction of 0.04 in bottom sediment. Measured organic carbon in bottom sediment, specific to site conditions, should be used to calculate Kd_{bs}, because the value varies, depending on the fraction of organic carbon in bottom sediment. Recommended Kd_{bs} value was calculated by using the K_{oc} value that is provided in this table.	B-4-16; B-4-25	8.10E+02

TABLE A-3-187

CHEMICAL-SPECIFIC INPUTS FOR 1,2,3-TRICHLOROBENZENE (87-61-6)

Parameter	Reference and Explanation	Equations	Value
Chemical/Physical Properties (Continued)			
ksg $(year)^{-1}$	*Ksg* value was calculated by using the chemical half-life in soil, as cited in Mackay, Shiu, and Ma (1992).	B-1-1; B-1-2; B-2-1; B-2-2; B-3-1; B-3-2; B-4-1; B-4-2	1.41E+00
Fv (unitless)	*Fv* value was calculated by using equations cited in Junge (1977) and Bidleman (1988). Recommended value of *Fv* was calculated by using T_m and *Vp* values that are provided in this table. *Vp* value for this compound was converted to a liquid-phase value before being used in the calculations.	B-1-1; B-2-1; B-2-7; B-2-8; B-3-1; B-3-7; B-3-8; B-4-1; B-4-8; B-4-9; B-4-12; B-5-1	1.00
Biotransfer Factors for Plants			
RCF $(\frac{\mu g/g\ DW\ plant}{\mu g/mL\ soil\ water})$	*RCF* value was calculated by using the correlation equation with K_{ow} that is cited in Briggs (1982). Recommended value was calculated by using the K_{ow} value that is provided in this table. The value was then converted to a dry weight basis by using a moisture content of 87 percent.	--	3.09E+02
$Br_{root\ veg}$ $(\frac{\mu g/g\ DW\ plant}{\mu g/g\ soil})$	$Br_{root\ veg}$ value was calculated by dividing the *RCF* value with the Kd_s value provided in this table.	B-2-10	1.53E+00
Br_{ag} $(\frac{\mu g/g\ DW\ plant}{\mu g/g\ soil})$	Br_{ag} value was calculated by using the correlation equation with K_{ow} that is cited in Travis and Arms (1988). No distinction was made between values for aboveground produce and forage. Recommended value was calculated by using the K_{ow} value that is provided in this table.	B-2-9	1.78E-01
Br_{forage} $(\frac{\mu g/g\ DW\ plant}{\mu g/g\ soil})$	Br_{forage} value was calculated by using the correlation equation with K_{ow} that is cited in Travis and Arms (1988). No distinction was made between values for abovegroud produce and forage. Recommended value was calculated by using the K_{ow} value that is provided in this table.	B-3-9	1.78E-01
Bv_{ag} $(\frac{\mu g/g\ DW\ plant}{\mu g/g\ air})$	Bv_{ag} value was calculated by using the correlation equation with K_{ow} and *H* that is cited in Bacci, Calamari, Gaggi, and Vighi (1990); and Bacci, Cerejeira, Gaggi, Chemello, Calamari, and Vighi (1992); then reducing this value by a factor of 100. No distinction was made between values for aboveground produce and forage. Recommended value was calculated, for a temperature (T) of 25°C, by using the *H* and K_{ow} values that are provided in this table.	B-2-8	4.01E-01
Bv_{forage} $(\frac{\mu g/g\ DW\ plant}{\mu g/g\ air})$	Bv_{forage} value was calculated by using the correlation equation with K_{ow} and *H* that is cited in Bacci, Calamari, Gaggi, and Vighi (1990); and Bacci, Cerejeira, Gaggi, Chemello, Calamari, and Vighi (1992); then reducing this value by a factor of 100. No distinction was made between values for aboveground produce and forage. Recommended value was calculated, for a temperature (T) of 25°C, by using the *H* and K_{ow} values that are provided in this table.	B-3-8	4.01E-01
Biotransfer Factors for Animals			
Ba_{milk} (day/kg FW)	Ba_{milk} value was calculated by using the correlation equation with K_{ow} that is cited in Travis and Arms (1988). Recommended value was calculated by using the K_{ow} value that is provided in this table.	B-3-11	8.82E-05

TABLE A-3-187

CHEMICAL-SPECIFIC INPUTS FOR 1,2,3-TRICHLOROBENZENE (87-61-6)

Parameter	Reference and Explanation	Equations	Value
Ba_{beef} (day/kg FW)	Ba_{beef} value was calculated by using the correlation equation with K_{ow} that is cited in Travis and Arms (1988). Recommended value was calculated by using the K_{ow} value that is provided in this table.	B-3-10	2.79E-04
Ba_{pork} (day/kg FW)	Ba_{pork} value was calculated by using the fat content ratio of pork to beef (23/19) and multiplying it with the Ba_{beef} value.	B-3-12	3.38E-04
Ba_{egg} (day/kg FW)	Ba_{egg} value was calculated by using the correlation equation with K_{ow} that is cited in California EPA (1993). Recommended value was calculated by using the K_{ow} value that is provided in this table.	B-3-13	8.82E-02
$Ba_{chicken}$ (day/kg FW)	$Ba_{chicken}$ value was calculated by using the fat content ratio of chicken to beef (15/19) and multiplying it with the Ba_{beef} value.	B-3-14	2.20E-04
BCF_{fish} (L/kg FW tissue)	--	B-4-26	NA
BAF_{fish} (L/kg FW)	*BAF*s were used for compounds with a log K_{ow} value above 4.0, as cited in U.S. EPA (1995b). *BAF* values were predicted values calculated by multiplying a food chain multiplier (*FCM*) with an estimated *BCF*. *BCF*s were estimated using the correlation equation obtained from Veith, Macek, Petrocelli, and Caroll (1980). *FCM*s were obtained from U.S. EPA (1995bc)—See Appendix A-3.	B-4-27	8.76E+02
$BSAF_{fish}$ (unitless)	--	B-4-28	NA
Health Benchmarks			
RfD (mg/kg/day)	--	C-1-8	ND
Oral CSF $(mg/kg/day)^{-1}$	--	C-1-7	ND
RfC (mg/m^3)	--	C-2-3	ND
Inhalation URF $(\mu g/m^3)^{-1}$	--	C-2-1	ND
Inhalation CSF $(mg/kg/day)^{-1}$	--	C-2-2	ND

Note:

NA = Not applicable
ND = No data available

All parameters are defined in list of FATE AND TRANSPORT PARAMETERS on page A-3-iii.

TABLE A-3-188

CHEMICAL-SPECIFIC INPUTS FOR 1,2,4-TRICHLOROBENZENE (120-82-1)

Parameter	Reference and Explanation	Equations	Value
Chemical/Physical Properties			
MW (g/mole)	Budavari, O'Neil, Smith, and Heckelman (1989)	--	181.46
T_m (K)	Budavari, O'Neil, Smith, and Heckelman (1989)	--	290.1
Vp (atm)	Geometric mean value cited in U.S. EPA (1994c)	--	4.42E-04 at 25°C (liquid)
S (mg/L)	Geometric mean value cited in U.S. EPA (1994c)	--	3.07E+01
H (atm·m^3/mol)	*H* value was calculated by using the theoretical equation from Lyman, Reehl, and Rosenblatt (1982), which defines the constant. Recommended value was calculated by using the *MW*, *S*, and *Vp* values that are provided in this table.	B-1-6; B-2-6; B-2-8; B-3-6; B-4-6; B-4-12; B-4-19	2.61E-03
D_a (cm^2/s)	D_a value was obtained from CHEMDAT8 database (U.S. EPA 1994d).	B-1-6; B-2-6; B-3-6; B-4-6; B-4-21	3.00E-02
D_w (cm^2/s)	D_w value was obtained from CHEMDAT8 database (U.S. EPA 1994d).	B-4-20	8.23E-06
K_{ow} (unitless)	Geometric mean value cited in U.S. EPA (1994c)	--	9.73E+03
K_{oc} (mL/g)	Geometric mean of measured values obtained from U.S. EPA (1996b).	--	1.66E+03
Kd_s (cm^3/g)	Kd_s value was calculated by using the correlation equation with K_{oc} that is cited in U.S. EPA (1993d) for an assumed organic carbon fraction of 0.01 in soil. Measured organic carbon in soil, specific to site conditions, should be used to calculate Kd_s, because the value varies, depending on the fraction of organic carbon in soil. Recommended Kd_s value was calculated by using the K_{oc} value that is provided in this table.	B-1-3; B-1-4; B-1-5; B-1-6; B-2-3; B-2-4; B-2-5; B-2-6; B-2-10; B-3-3; B-3-4; B-3-5; B-3-6; B-4-3; B-4-4; B-4-5; B-4-6; B-4-10; B-4-11	1.66E+01
Kd_{sw} (L/Kg)	Kd_{sw} value was calculated by using the correlation equation with K_{oc} that is cited in U.S. EPA (1993d) for an assumed organic carbon fraction of 0.075 in suspended sediment. Measured organic carbon in suspended sediment, specific to site conditions, should be used to calculate Kd_{sw}, because the value varies, depending on the fraction of organic carbon in suspended sediment. Recommended Kd_{sw} value was calculated by using the K_{oc} value that is provided in this table.	B-4-16; B-4-18; B-4-24	1.24E+02
Kd_{bs} (cm^3/g)	Kd_{bs} value was calculated by using the correlation equation with K_{oc} that is cited in U.S. EPA (1993d) for an assumed organic carbon fraction of 0.04 in bottom sediment. Measured organic carbon in bottom sediment, specific to site conditions, should be used to calculate Kd_{bs}, because the value varies, depending on the fraction of organic carbon in bottom sediment. Recommended Kd_{bs} value was calculated by using the K_{oc} value that is provided in this table.	B-4-16; B-4-25	6.64E+01
Chemical/Physical Properties (Continued)			
ksg (year)$^{-1}$	*ksg* value was calculated by using the chemical half-life in soil, as cited in Howard, Boethling, Jarvis, Meylan, and Michalenko (1991) and Mackay, Shiu, and Ma (1992).	B-1-2; B-2-2; B-3-2; B-4-2	1.41E+00
Fv (unitless)	*Fv* value was calculated by using the equation cited in Junge (1977). Recommended value of *Fv* was calculated by using the *Vp* value that is provided in this table.	B-1-1; B-2-1; B-2-7; B-2-8; B-3-1; B-3-7;	1.0

TABLE A-3-188

CHEMICAL-SPECIFIC INPUTS FOR 1,2,4-TRICHLOROBENZENE (120-82-1)

Parameter	Reference and Explanation	Equations	Value
Biotransfer Factors for Plants			
RCF ($\frac{\mu g/g\ DW\ plant}{\mu g/mL\ soil\ water}$)	*RCF* value was calculated by using the correlation equation with K_{ow} that is cited in Briggs (1982). Recommended value was calculated by using the K_{ow} value that is provided in this table. The value was then converted to a dry weight basis by using a moisture content of 87 percent.	B-2-10	2.80E+02
$Br_{root\ veg}$ ($\frac{\mu g/g\ DW\ plant}{\mu g/g\ soil}$)	$Br_{root\ veg}$ value was calculated by dividing the *RCF* value with the Kd_s value provided in this table.	B-2-10	1.69E+01
Br_{ag} ($\frac{\mu g/g\ DW\ plant}{\mu g/g\ soil}$)	Br_{ag} value was calculated by using the correlation equation with K_{ow} that is cited in Travis and Arms (1988). No distinction was made between values for aboveground produce and forage. Recommended value was calculated by using the K_{ow} value that is provided in this table.	B-2-9	1.92E-01
Br_{forage} ($\frac{\mu g/g\ DW\ plant}{\mu g/g\ soil}$)	Br_{forage} value was calculated by using the correlation equation with K_{ow} that is cited in Travis and Arms (1988). No distinction was made between values for aboveground produce and forage. Recommended value was calculated by using the K_{ow} value that is provided in this table.	B-3-9	1.92E-01
Bv_{ag} ($\frac{\mu g/g\ DW\ plant}{\mu g/g\ air}$)	Bv_{ag} value was calculated by using the correlation equation with K_{ow} and *H* that is cited in Bacci, Calamari, Gaggi, and Vighi (1990); and Bacci, Cerejeira, Gaggi, Chemello, Calamari, and Vighi (1992); then reducing this value by a factor of 100. No distinction was made between values for aboveground produce and forage. Recommended value was calculated, for a temperature (T) of 25°C, by using the *H* and K_{ow} values that are provided in this table.	B-2-8	3.78E-01
Bv_{forage} ($\frac{\mu g/g\ DW\ plant}{\mu g/g\ air}$)	Bv_{forage} value was calculated by using the correlation equation with K_{ow} and *H* that is cited in Bacci, Calamari, Gaggi, and Vighi (1990); and Bacci, Cerejeira, Gaggi, Chemello, Calamari, and Vighi (1992); then reducing this value by a factor of 100. No distinction was made between values for aboveground produce and forage. Recommended value was calculated, for a temperature (T) of 25°C, by using the *H* and K_{ow} values that are provided in this table.	B-3-8	3.78E-01
Biotransfer Factors for Animals			
Ba_{milk} (day/kg FW)	Ba_{milk} value was calculated by using the correlation equation with K_{ow} that is cited in Travis and Arms (1988). Recommended value was calculated by using the K_{ow} value that is provided in this table.	B-3-11	7.73E-05
Ba_{beef} (day/kg FW)	Ba_{beef} value was calculated by using the correlation equation with K_{ow} that is cited in Travis and Arms (1988). Recommended value was calculated by using the K_{ow} value that is provided in this table.	B-3-10	2.45E-04
Ba_{pork} (day/kg FW)	Ba_{pork} value was calculated by using the fat content ratio of pork to beef (23/19) and multiplying it with the Ba_{beef} value.	B-3-12	2.96E-04
Ba_{eggs} (day/kg FW)	Ba_{eggs} value was calculated by using the correlation equation with K_{ow} that is cited in California EPA (1993). Recommended value was calculated by using the K_{ow} value that is provided in this table.	B-3-13	7.73E-02
$Ba_{chicken}$ (day/kg FW)	$Ba_{chicken}$ value was calculated by using the fat content ratio of chicken to beef (15/19) and multiplying it with the Ba_{beef} value.	B-3-14	1.93E-04

TABLE A-3-188

CHEMICAL-SPECIFIC INPUTS FOR 1,2,4-TRICHLOROBENZENE (120-82-1)

Parameter	Reference and Explanation	Equations	Value
BCF_{fish} (L/kg FW tissue)	*BCFs* were used for compounds with a log K_{ow} value below 4.0, as cited in U.S. EPA (1995b). BCF_{fish} value calculated using the correlation equation with K_{ow} obtained from Veith, Macek, Petrocelli, and Caroll (1980)—See Appendix A-3.	B-4-26	6.33E+02
BAF_{fish} (L/kg FW)	--	B-4-27	NA
$BSAF_{fish}$ (unitless)	--	B-4-28	NA
Health Benchmarks			
RfD (mg/kg/day)	U.S. EPA (1997b)	C-1-8	1.0E-02
Oral CSF $(mg/kg/day)^{-1}$	--	C-1-7	ND
RfC (mg/m^3)	U.S. EPA (1997c)	C-2-3	2.0E-01
Inhalation URF $(\mu g/m^3)^{-1}$	--	C-2-1	ND
Inhalation CSF $(mg/kg/day)^{-1}$	--	C-2-2	ND

Note:

NA= Not applicable
ND= No data available

All parameters are defined in list of FATE AND TRANSPORT PARAMETERS on page A-3-iii.

TABLE A-3-189

CHEMICAL-SPECIFIC INPUTS FOR 1,1,1-TRICHLOROETHANE (71-55-6)

Parameter	Reference and Explanation	Equations	Value
Chemical/Physical Properties			
MW (g/mole)	Budavari, O'Neil, Smith, and Heckelman (1989)	--	133.42
T_m (K)	Budavari, O'Neil, Smith, and Heckelman (1989)	--	242.7
Vp (atm)	Geometric mean value cited in U.S. EPA (1994c)	--	1.63E-01 at 25°C (liquid)
S (mg/L)	Geometric mean value cited in U.S. EPA (1994c)	--	1.17E+03
H (atm·m^3/mol)	*H* value was calculated by using the theoretical equation from Lyman, Reehl, and Rosenblatt (1982), which defines the constant. Recommended value was calculated by using the *MW*, *S*, and *Vp* values that are provided in this table.	B-1-6; B-2-6; B-2-8; B-3-6; B-4-6; B-4-12; B-4-19	1.86E-02
D_a (cm^2/s)	D_a value was obtained from CHEMDAT8 database (U.S. EPA 1994d).	B-1-6; B-2-6; B-3-6; B-4-6; B-4-21	4.66E-02
D_w (cm^2/s)	D_w value was obtained from CHEMDAT8 database (U.S. EPA 1994d).	B-4-20	9.56E-06
K_{ow} (unitless)	Geometric mean value cited in U.S. EPA (1994c)	--	2.64E+02
K_{oc} (mL/g)	Geometric mean value cited in U.S. EPA (1996b)	--	1.35E+05
Kd_s (cm^3/g)	Kd_s value was calculated by using the correlation equation with K_{oc} that is cited in U.S. EPA (1993d) for an assumed organic carbon fraction of 0.01 in soil. Measured organic carbon in soil, specific to site conditions, should be used to calculate Kd_s, because the value varies, depending on the fraction of organic carbon in soil. Recommended Kd_s value was calculated by using the K_{oc} value that is provided in this table.	B-1-3; B-1-4; B-1-5; B-1-6; B-2-3; B-2-4; B-2-5; B-2-6; B-3-3; B-3-4; B-3-5; B-3-6; B-4-3; B-4-4; B-4-5; B-4-6; B-4-10; B-4-11	1.35E+03
Kd_{sw} (L/Kg)	Kd_{sw} value was calculated by using the correlation equation with K_{oc} that is cited in U.S. EPA (1993d) for an assumed organic carbon fraction of 0.075 in suspended sediment. Measured organic carbon in suspended sediment, specific to site conditions, should be used to calculate Kd_{sw}, because the value varies, depending on the fraction of organic carbon in suspended sediment. Recommended Kd_{sw} value was calculated by using the K_{oc} value that is provided in this table.	B-4-16; B-4-18; B-4-24	1.01E+04
Kd_{bs} (cm^3/g)	Kd_{bs} value was calculated by using the correlation equation with K_{oc} that is cited in U.S. EPA (1993d) for an assumed organic carbon fraction of 0.04 in bottom sediment. Measured organic carbon in bottom sediment, specific to site conditions, should be used to calculate Kd_{bs}, because the value varies, depending on the fraction of organic carbon in bottom sediment. Recommended Kd_{bs} value was calculated by using the K_{oc} value that is provided in this table.	B-4-16; B-4-25	5.40E+03
Chemical/Physical Properties (Continued)			
ksg (year)$^{-1}$	*Ksg* value was calculated by using the chemical half-life in soil, as cited in Howard, Boethling, Jarvis, Meylan, and Michalenko (1991).	B-1-1; B-1-2; B-2-1; B-2-2; B-3-1; B-3-2; B-4-1; B-4-2	9.26E-01
Fv (unitless)	*Fv* value was calculated by using the equation cited in Junge (1977). Recommended value of *Fv* was calculated by using the *Vp* value that is provided	B-1-1; B-2-1; B-2-7; B-2-8;	1.00

TABLE A-3-189

CHEMICAL-SPECIFIC INPUTS FOR 1,1,1-TRICHLOROETHANE (71-55-6)

Parameter	Reference and Explanation	Equations	Value
Biotransfer Factors for Plants			
RCF $(\frac{\mu g/g\ DW\ plant}{\mu g/mL\ soil\ water})$	*RCF* value was calculated by using the correlation equation with K_{ow} that is cited in Briggs (1982). Recommended value was calculated by using the K_{ow} value that is provided in this table. The value was then converted to a dry weight basis by using a moisture content of 87 percent.	--	2.33E+01
$Br_{root\ veg}$ $(\frac{\mu g/g\ DW\ plant}{\mu g/g\ soil})$	$Br_{root\ veg}$ value was calculated by dividing the *RCF* value with the Kd_s value provided in this table.	B-2-10	1.73E-02
Br_{ag} $(\frac{\mu g/g\ DW\ plant}{\mu g/g\ soil})$	Br_{ag} value was calculated by using the correlation equation with K_{ow} that is cited in Travis and Arms (1988). No distinction was made between values for aboveground produce and forage. Recommended value was calculated by using the K_{ow} value that is provided in this table.	B-2-9	1.54E+00
Br_{forage} $(\frac{\mu g/g\ DW\ plant}{\mu g/g\ soil})$	Br_{forage} value was calculated by using the correlation equation with K_{ow} that is cited in Travis and Arms (1988). No distinction was made between values for abovegroud produce and forage. Recommended value was calculated by using the K_{ow} value that is provided in this table.	B-3-9	1.54E+00
Bv_{ag} $(\frac{\mu g/g\ DW\ plant}{\mu g/g\ air})$	Bv_{ag} value was calculated by using the correlation equation with K_{ow} and *H* that is cited in Bacci, Calamari, Gaggi, and Vighi (1990); and Bacci, Cerejeira, Gaggi, Chemello, Calamari, and Vighi (1992); then reducing this value by a factor of 100. No distinction was made between values for aboveground produce and forage. Recommended value was calculated, for a temperature (T) of 25ºC, by using the *H* and K_{ow} values that are provided in this table.	B-2-8	1.14E-03
Bv_{forage} $(\frac{\mu g/g\ DW\ plant}{\mu g/g\ air})$	Bv_{forage} value was calculated by using the correlation equation with K_{ow} and *H* that is cited in Bacci, Calamari, Gaggi, and Vighi (1990); and Bacci, Cerejeira, Gaggi, Chemello, Calamari, and Vighi (1992); then reducing this value by a factor of 100. No distinction was made between values for aboveground produce and forage. Recommended value was calculated, for a temperature (T) of 25ºC, by using the *H* and K_{ow} values that are provided in this table.	B-3-8	1.14-03
Biotransfer Factors for Animals			
Ba_{milk} (day/kg FW)	Ba_{milk} value was calculated by using the correlation equation with K_{ow} that is cited in Travis and Arms (1988). Recommended value was calculated by using the K_{ow} value that is provided in this table.	B-3-11	2.10E-06
Ba_{beef} (day/kg FW)	Ba_{beef} value was calculated by using the correlation equation with K_{ow} that is cited in Travis and Arms (1988). Recommended value was calculated by using the K_{ow} value that is provided in this table.	B-3-10	6.63E-06
Ba_{pork} (day/kg FW)	Ba_{pork} value was calculated by using the fat content ratio of pork to beef (23/19) and multiplying it with the Ba_{beef} value.	B-3-12	8.03E-06
Ba_{egg} (day/kg FW)	Ba_{egg} value was calculated by using the correlation equation with K_{ow} that is cited in California EPA (1993). Recommended value was calculated by using the K_{ow} value that is provided in this table.	B-3-13	2.10E-03
$Ba_{chicken}$ (day/kg FW)	$Ba_{chicken}$ value was calculated by using the fat content ratio of chicken to beef (15/19) and multiplying it with the Ba_{beef} value.	B-3-14	5.24E-06

TABLE A-3-189

CHEMICAL-SPECIFIC INPUTS FOR 1,1,1-TRICHLOROETHANE (71-55-6)

Parameter	Reference and Explanation	Equations	Value
BCF_{fish} (L/kg FW tissue)	*BCFs* were used for compounds with a log K_{ow} value below 4.0, as cited in U.S. EPA (1995b). BCF_{fish} value calculated using the correlation equation with K_{ow} obtained from Veith, Macek, Petrocelli, and Caroll (1980)—See Appendix A-3.	B-4-26	4.08E+01
BAF_{fish} (L/kg FW)	--	B-4-27	NA
$BSAF_{fish}$ (unitless)	--	B-4-28	NA
Health Benchmarks			
RfD (mg/kg/day)	U.S. EPA (1997a)	C-1-8	3.50E-02
Oral CSF $(mg/kg/day)^{-1}$	--	C-1-7	NA
RfC (mg/m^3)	Calculated from *RfD* using an inhalation rate of 20 m^3/day and a human body weight of 70 kg.	C-2-3	1.23E-01
Inhalation URF $(\mu g/m^3)^{-1}$	--	C-2-1	NA
Inhalation CSF $(mg/kg/day)^{-1}$	--	C-2-2	NA

Note:

NA = Not applicable
ND = No data available

All parameters are defined in list of FATE AND TRANSPORT PARAMETERS on page A-3-iii.

TABLE A-3-190

CHEMICAL-SPECIFIC INPUTS FOR 1,1,2-TRICHLOROETHANE (79-00-5)

Parameter	Reference and Explanation	Equations	Value
Chemical/Physical Properties			
MW (g/mole)	Budavari, O'Neil, Smith, and Heckelman (1989)	--	133.42
T_m (K)	Budavari, O'Neil, Smith, and Heckelman (1989)	--	238.1
Vp (atm)	Geometric mean value cited in U.S. EPA (1994c).	--	3.31E-02 at 25°C (liquid)
S (mg/L)	Geometric mean value cited in U.S. EPA (1994c).	--	4.40E+03
H (atm·m^3/mol)	*H* value was calculated by using the theoretical equation from Lyman, Reehl, and Rosenblatt (1982), which defines the constant. Recommended value was calculated by using the *MW*, *S*, and *Vp* values that are provided in this table.	B-1-6; B-2-6; B-2-8; B-3-6; B-4-6; B-4-12; B-4-19	1.00E-03
D_a (cm^2/s)	D_a value was obtained from CHEMDAT8 database (U.S. EPA 1994d).	B-1-6; B-2-6; B-3-6; B-4-6; B-4-21	4.51E-02
D_w (cm^2/s)	D_w value was obtained from CHEMDAT8 database (U.S. EPA 1994d).	B-4-20	1.0E-05
K_{ow} (unitless)	Geometric mean value cited in U.S. EPA (1994c).	--	1.25E+02
K_{oc} (mL/g)	Geometric mean of measured values obtained from U.S. EPA (1996b).	--	7.50E+01
Kd_s (cm^3/g)	Kd_s value was calculated by using the correlation equation with K_{oc} that is cited in U.S. EPA (1993d) for an assumed fraction organic carbon of 0.01 in soil. Measured organic carbon in soil, specific to site conditions, should be used to calculate Kd_s, because the value varies, depending on the fraction of organic carbon in soil. Recommended Kd_s value was calculated by using the K_{oc} value that is provided in this table.	B-1-3; B-1-4; B-1-5; B-1-6; B-2-3; B-2-4; B-2-5; B-2-6; B-2-10; B-3-3; B-3-4; B-3-5; B-3-6; B-4-3; B-4-4; B-4-5; B-4-6; B-4-10; B-4-11	7.50E-01
Kd_{sw} (L/Kg)	Kd_{sw} value was calculated by using the correlation equation with K_{oc} that is cited in U.S. EPA (1993d) for an assumed organic carbon fraction of 0.075 in suspended sediment. Measured organic carbon in suspended sediment, specific to site conditions, should be used to calculate Kd_{sw}, because the value varies, depending on the fraction of organic carbon in suspended sediment. Recommended Kd_{sw} value was calculated by using the K_{oc} value that is provided in this table.	B-4-16; B-4-18; B-4-24	5.63E+00
Kd_{bs} (cm^3/g)	Kd_{bs} value was calculated by using the correlation equation with K_{oc} that is cited in U.S. EPA (1993d) for an assumed organic carbon of 0.04 in bottom sediment. Measured organic carbon in bottom sediment, specific to site conditions, should be used to calculate Kd_{bs}, because the value varies depending on the fraction of organic fraction in bottom sediment. Recommended Kd_{bs} value was calculated by using the K_{oc} value that is provided in this table.	B-4-16; B-4-25	3.00E+00

TABLE A-3-190

CHEMICAL-SPECIFIC INPUTS FOR 1,1,2-TRICHLOROETHANE (79-00-5)

Parameter	Reference and Explanation	Equations	Value
Chemical/Physical Properties (Continued)			
ksg $(year)^{-1}$	*Ksg* value was calculated by using the chemical half-life in soil, as cited in Howard, Boethling, Jarvis, Meylan, and Michalenko (1991).	B-1-2; B-2-2; B-3-2; B-4-2	6.93E-01
Fv (unitless)	*Fv* value was calculated by using the equation cited in Junge (1977). Recommended value of *Fv* was calculated by using the *Vp* value that is provided in this table.	B-1-1; B-2-1; B-2-7; B-2-8; B-3-1; B-3-7; B-3-8; B-4-1; B-4-8; B-4-9; B-4-12; B-5-1	1.0
Biotransfer Factors for Plants			
RCF $(\frac{\mu g/g\ DW\ plant}{\mu g/mL\ soil\ water})$	*RCF* value was calculated by using the correlation equation with K_{ow} that is cited in Briggs (1982). Recommended value was calculated by using the K_{ow} value that is provided in this table. The value was converted to a dry weight basis by using a moisture content of 87 percent.	B-2-10	1.59E+01
$Br_{root\ veg}$ $(\frac{\mu g/g\ DW\ plant}{\mu g/g\ soil})$	$Br_{root\ veg}$ value was calculated by dividing the *RCF* value with the Kd_s value provided in this table (see section A3.4.2 of Appendix A-3).	B-2-10	2.12E+01
Br_{ag} $(\frac{\mu g/g\ DW\ plant}{\mu g/g\ soil})$	Br_{ag} value was calculated by using the correlation equation with K_{ow} that is cited in Travis and Arms (1988). No distinction was made between values for aboveground produce and forage. Recommended value was calculated by using the K_{ow} value that is provided in this table.	B-2-9	2.38E+00
Br_{forage} $(\frac{\mu g/g\ DW\ plant}{\mu g/g\ soil})$	Br_{forage} value was calculated by using the correlation equation with K_{ow} that is cited in Travis and Arms (1988). No distinction was made between values for aboveground produce and forage. Recommended value was calculated by using the K_{ow} value that is provided in this table.	B-3-9	2.38E+00
Bv_{ag} $(\frac{\mu g/g\ DW\ plant}{\mu g/g\ air})$	Bv_{ag} value was calculated by using the correlation equation with K_{ow} and *H* that is cited in Bacci, Calamari, Gaggi, and Vighi (1990); and Bacci, Cerejeira, Gaggi, Chemello, Calamari, and Vighi (1992); then reducing this value by a factor of 100, as recommended by U.S. EPA (1993d). No distinction was made between values for aboveground produce and forage. Recommended value was calculated, for a temperature (T) of 25ºC, by using the *H* and K_{ow} values that are provided in this table.	B-2-8	9.53E-03
Bv_{forage} $(\frac{\mu g/g\ DW\ plant}{\mu g/g\ air})$	Bv_{forage} value was calculated by using the correlation equation with K_{ow} and *H* that is cited in Bacci, Calamari, Gaggi, and Vighi (1990); and Bacci, Cerejeira, Gaggi, Chemello, Calamari, and Vighi (1992); then reducing this value by a factor of 100, as recommended by U.S. EPA (1993d). No distinction was made between values for aboveground produce and forage. Recommended value was calculated, for a temperature (T) of 25ºC, by using the *H* and K_{ow} values that are provided in this table.	B-3-8	9.53E-03
Biotransfer Factors for Animals			
Ba_{milk} (day/kg FW)	Ba_{milk} value was calculated by using the correlation equation with K_{ow} that is cited in Travis and Arms (1988). Recommended value was calculated by using the K_{ow} value that is provided in this table.	B-3-11	9.93E-07

TABLE A-3-190

CHEMICAL-SPECIFIC INPUTS FOR 1,1,2-TRICHLOROETHANE (79-00-5)

Parameter	Reference and Explanation	Equations	Value
Ba_{beef} (day/kg FW)	Ba_{beef} value was calculated by using the correlation equation with K_{ow} that is cited in Travis and Arms (1988). Recommended value was calculated by using the K_{ow} value that is provided in this table.	B-3-10	3.14E-06
Ba_{pork} (day/kg FW)	Ba_{pork} value was calculated by using the fat content ratio of pork to beef (23/19) and multiplying it with the Ba_{beef} value (see section A3.4.2 of Appendix A-3).	B-3-12	3.80E-06
Ba_{egg} (day/kg FW)	Ba_{egg} value was calculated by using the correlation equation with K_{ow} that is cited in California EPA (1993). Recommended value was calculated by using the K_{ow} value that is provided in this table.	B-3-13	9.93E-04
$Ba_{chicken}$ (day/kg FW)	$Ba_{chicken}$ value was calculated by using the fat content ratio of chicken to beef (15/19) and multiplying it with the Ba_{beef} value (see section A3.4.3 of Appendix A-3).	B-3-14	2.48E-06
BCF_{fish} (L/kg FW tissue)	*BCFs* were used for compounds with a log K_{ow} value below 4.0, as cited in U.S. EPA (1995b). BCF_{fish} value calculated using the correlation equation with K_{ow} obtained from Veith, Macek, Petrocelli, and Caroll (1980)—See Appendix A-3.	B-4-26	2.31E+01
BAF_{fish} (L/kg FW)	--	B-4-27	NA
$BSAF_{fish}$ (unitless)	--	B-4-28	NA
Health Benchmarks			
RfD (mg/kg/day)	U.S. EPA (1997b)	C-1-8	4.0E-03
Oral CSF $(mg/kg/day)^{-1}$	U.S. EPA (1997b)	C-1-7	5.70E-02
RfC (mg/m^3)	Calculated from *RfD* using an inhalation rate of 20 m^3/day and a human body weight of 70 kg.	C-2-3	1.4E-02
Inhalation URF $(\mu g/m^3)^{-1}$	U.S. EPA (1997b)	C-2-1	1.6E-05
Inhalation CSF $(mg/kg/day)^{-1}$	U.S. EPA (1997c)	C-2-2	5.7E-02

Note:

NA = Not applicable
ND = No data available

All parameters are defined in list of FATE AND TRANSPORT PARAMETERS on page A-3-iii.

TABLE A-3-191

CHEMICAL-SPECIFIC INPUTS FOR TRICHLOROETHYLENE (79-01-6)

Parameter	Reference and Explanation	Equations	Value
Chemical/Physical Properties			
MW (g/mole)	Budavari, O'Neil, Smith, and Heckelman (1989)	--	131.40
T_m (K)	Budavari, O'Neil, Smith, and Heckelman (1989)	--	188.3
Vp (atm)	Geometric mean value cited in U.S. EPA (1994c).	--	9.48E-02 at 25°C (liquid)
S (mg/L)	Geometric mean value cited in U.S. EPA (1994c).	--	1.18E+03
H (atm·m^3/mol)	*H* value was calculated by using the theoretical equation from Lyman, Reehl, and Rosenblatt (1982), which defines the constant. Recommended value was calculated by using the *MW*, *S*, and *Vp* values that are provided in this table.	B-1-6; B-2-6; B-2-8; B-3-6; B-4-6; B-4-12; B-4-19	1.06E-02
D_a (cm^2/s)	D_a value was obtained from CHEMDAT8 database (U.S. EPA 1994d).	B-1-6; B-2-6; B-3-6; B-4-6; B-4-21	4.65E-02
D_w (cm^2/s)	D_w value was obtained from CHEMDAT8 database (U.S. EPA 1994d).	B-4-20	9.94E-06
K_{ow} (unitless)	Geometric mean value cited in U.S. EPA (1994c).	--	2.71E+02
K_{oc} (mL/g)	K_{oc} value was calculated by using the correlation equation with K_{ow} for all nonionizing organics except phthalates, PAHs, dioxins, and furans as cited in U.S. EPA (1994c). K_{oc} value was calculated by using the recommended K_{ow} value that is provided in this table.	--	9.40E+01
Kd_s (cm^3/g)	Kd_s value was calculated by using the correlation equation with K_{oc} that is cited in U.S. EPA (1993d) for an assumed fraction organic carbon of 0.01 in soil. Measured organic carbon in soil, specific to site conditions, should be used to calculate Kd_s, because the value varies, depending on the fraction of organic carbon in soil. Recommended Kd_s value was calculated by using the K_{oc} value that is provided in this table.	B-1-3; B-1-4; B-1-5; B-1-6; B-2-3; B-2-4; B-2-5; B-2-6; B-2-10; B-3-3; B-3-4; B-3-5; B-3-6; B-4-3; B-4-4; B-4-5; B-4-6; B-4-10; B-4-11	9.40E-01
Kd_{sw} (L/Kg)	Kd_{sw} value was calculated by using the correlation equation with K_{oc} that is cited in U.S. EPA (1993d) for an assumed organic carbon fraction of 0.075 in suspended sediment. Measured organic carbon in suspended sediment, specific to site conditions, should be used to calculate Kd_{sw}, because the value varies, depending on the fraction of organic carbon in suspended sediment. Recommended Kd_{sw} value was calculated by using the K_{oc} value that is provided in this table.	B-4-16; B-4-18; B-4-24	7.05E+00
Kd_{bs} (cm^3/g)	Kd_{bs} value was calculated by using the correlation equation with K_{oc} that is cited in U.S. EPA (1993d) for an assumed organic carbon of 0.04 in bottom sediment. Measured organic carbon in bottom sediment, specific to site conditions, should be used to calculate Kd_{bs}, because the value varies depending on the fraction of organic fraction in bottom sediment. Recommended Kd_{bs} value was calculated by using the K_{oc} value that is provided in this table.	B-4-16; B-4-25	3.76E+00

TABLE A-3-191

CHEMICAL-SPECIFIC INPUTS FOR TRICHLOROETHYLENE (79-01-6)

Parameter	Reference and Explanation	Equations	Value
Chemical/Physical Properties (Continued)			
ksg $(year)^{-1}$	*Ksg* value was calculated by using the chemical half-life in soil, as cited in Howard, Boethling, Jarvis, Meylan, and Michalenko (1991).	B-1-2; B-2-2; B-3-2; B-4-2	0.703
Fv (unitless)	*Fv* value was calculated by using the equation cited in Junge (1977). Recommended value of *Fv* was calculated by using the *Vp* value that is provided in this table.	B-1-1; B-2-1; B-2-7; B-2-8; B-3-1; B-3-7; B-3-8; B-4-1; B-4-8; B-4-9; B-4-12; B-5-1	1.0
Biotransfer Factors for Plants			
RCF $(\frac{\mu g/g\ DW\ plant}{\mu g/mL\ soil\ water})$	*RCF* value was calculated by using the correlation equation with K_{ow} that is cited in Briggs (1982). Recommended value was calculated by using the K_{ow} value that is provided in this table. The value was converted to a dry weight basis by using a moisture content of 87 percent.	B-2-10	2.37E+01
$Br_{root\ veg}$ $(\frac{\mu g/g\ DW\ plant}{\mu g/g\ soil})$	$Br_{root\ veg}$ value was calculated by dividing the *RCF* value with the Kd_s value provided in this table (see section A3.4.2 of Appendix A-3).	B-2-10	2.12E+01
Br_{ag} $(\frac{\mu g/g\ DW\ plant}{\mu g/g\ soil})$	Br_{ag} value was calculated by using the correlation equation with K_{ow} that is cited in Travis and Arms (1988). No distinction was made between values for aboveground produce and forage. Recommended value was calculated by using the K_{ow} value that is provided in this table.	B-2-9	1.52E+00
Br_{forage} $(\frac{\mu g/g\ DW\ plant}{\mu g/g\ soil})$	Br_{forage} value was calculated by using the correlation equation with K_{ow} that is cited in Travis and Arms (1988). No distinction was made between values for aboveground produce and forage. Recommended value was calculated by using the K_{ow} value that is provided in this table.	B-3-9	1.52E+00
Bv_{ag} $(\frac{\mu g/g\ DW\ plant}{\mu g/g\ air})$	Bv_{ag} value was calculated by using the correlation equation with K_{ow} and *H* that is cited in Bacci, Calamari, Gaggi, and Vighi (1990); and Bacci, Cerejeira, Gaggi, Chemello, Calamari, and Vighi (1992); then reducing this value by a factor of 100, as recommended by U.S. EPA (1993d). No distinction was made between values for aboveground produce and forage. Recommended value was calculated, for a temperature (T) of 25°C, by using the *H* and K_{ow} values that are provided in this table.	B-2-8	2.07E-03
Bv_{forage} $(\frac{\mu g/g\ DW\ plant}{\mu g/g\ air})$	Bv_{forage} value was calculated by using the correlation equation with K_{ow} and *H* that is cited in Bacci, Calamari, Gaggi, and Vighi (1990); and Bacci, Cerejeira, Gaggi, Chemello, Calamari, and Vighi (1992); then reducing this value by a factor of 100, as recommended by U.S. EPA (1993d). No distinction was made between values for aboveground produce and forage. Recommended value was calculated, for a temperature (T) of 25°C, by using the *H* and K_{ow} values that are provided in this table.	B-3-8	2.07E-03
Biotransfer Factors for Animals			
Ba_{milk} (day/kg FW)	Ba_{milk} value was calculated by using the correlation equation with K_{ow} that is cited in Travis and Arms (1988). Recommended value was calculated by using the K_{ow} value that is provided in this table.	B-3-11	2.15E-06

TABLE A-3-191

CHEMICAL-SPECIFIC INPUTS FOR TRICHLOROETHYLENE (79-01-6)

Parameter	Reference and Explanation	Equations	Value
Ba_{beef} (day/kg FW)	Ba_{beef} value was calculated by using the correlation equation with K_{ow} that is cited in Travis and Arms (1988). Recommended value was calculated by using the K_{ow} value that is provided in this table.	B-3-10	6.81E-06
Ba_{pork} (day/kg FW)	Ba_{pork} value was calculated by using the fat content ratio of pork to beef (23/19) and multiplying it with the Ba_{beef} value (see section A3.4.2 of Appendix A-3).	B-3-12	8.24E-06
Ba_{egg} (day/kg FW)	Ba_{egg} value was calculated by using the correlation equation with K_{ow} that is cited in California EPA (1993). Recommended value was calculated by using the K_{ow} value that is provided in this table.	B-3-13	2.15E-03
$Ba_{chicken}$ (day/kg FW)	$Ba_{chicken}$ value was calculated by using the fat content ratio of chicken to beef (15/19) and multiplying it with the Ba_{beef} value (see section A3.4.3 of Appendix A-3).	B-3-14	5.37E-06
BCF_{fish} (L/kg, FW tissue)	*BCFs* were used for compounds with a log K_{ow} value below 4.0, as cited in U.S. EPA (1995b). BCF_{fish} value calculated using the correlation equation with K_{ow} obtained from Veith, Macek, Petrocelli, and Caroll (1980)—See Appendix A-3.	B-4-26	4.16E+01
BAF_{fish} (L/kg FW)	--	B-4-27	NA
$BSAF_{fish}$ (unitless)	--	B-4-28	NA
Health Benchmarks			
RfD (mg/kg/day)	U.S.EPA (1997a)	C-1-8	6.0E-03
Oral CSF $(mg/kg/day)^{-1}$	U.S. EPA (1995b)	C-1-7	1.1E-02
RfC (mg/m^3)	Calculated from *RfD* using an inhalation rate of 20 m^3/day and a human body weight of 70 kg.	C-2-3	2.1E-02
Inhalation URF $(\mu g/m^3)^{-1}$	U.S. EPA (1995b)	C-2-1	1.7E-06
Inhalation CSF $(mg/kg/day)^{-1}$	Value based on *Oral CSF* assuming route-to-route extrapolation.	C-2-2	1.1E-02

Note:

NA = Not applicable
ND = No data available

All parameters are defined in list of FATE AND TRANSPORT PARAMETERS on page A-3-iii.

TABLE A-3-192

CHEMICAL-SPECIFIC INPUTS FOR TRICHLOROFLUOROMETHANE (75-69-4)

Parameter	Reference and Explanation	Equations	Value
Chemical/Physical Properties			
MW (g/mole)	Budavari, O'Neil, Smith, and Heckelman (1989)	--	137.38
T_m (K)	Budavari, O'Neil, Smith, and Heckelman (1989)	--	162.1
Vp (atm)	*Vp* value cited in U.S. EPA (1995b).	--	1.10E+00 at 25°C (liquid)
S (mg/L)	*S* value cited in U.S. EPA (1995b).	--	1.10E+03
H (atm·m^3/mol)	*H* value was calculated by using the theoretical equation from Lyman, Reehl, and Rosenblatt (1982), which defines the constant. Recommended value was calculated by using the *MW*, *S*, and *Vp* values that are provided in this table.	B-1-6; B-2-6; B-2-8; B-3-6; B-4-6; B-4-12; B-4-19	1.37E-01
D_a (cm^2/s)	D_a value was obtained from CHEMDAT8 database (U.S. EPA 1994d).	B-1-6; B-2-6; B-3-6; B-4-6; B-4-21	4.27E-02
D_w (cm^2/s)	D_w value was obtained from CHEMDAT8 database (U.S. EPA 1994d).	B-4-20	1.0E-05
K_{ow} (unitless)	K_{ow} value cited in U.S. EPA (1995b).	--	3.40E+02
K_{oc} (mL/g)	K_{oc} value was calculated by using the correlation equation with K_{ow} for all nonionizing organics except phthalates, PAHs, dioxins, and furans as cited in U.S. EPA (1994c). K_{oc} value was calculated by using the recommended K_{ow} value that is provided in this table.	--	1.34E+02
Kd_s (cm^3/g)	Kd_s value was calculated by using the correlation equation with K_{oc} that is cited in U.S. EPA (1993d) for an assumed fraction organic carbon of 0.01 in soil. Measured organic carbon in soil, specific to site conditions, should be used to calculate Kd_s, because the value varies, depending on the fraction of organic carbon in soil. Recommended Kd_s value was calculated by using the K_{oc} value that is provided in this table.	B-1-3; B-1-4; B-1-5; B-1-6; B-2-3; B-2-4; B-2-5; B-2-6; B-2-10; B-3-3; B-3-4; B-3-5; B-3-6; B-4-3; B-4-4; B-4-5; B-4-6; B-4-10; B-4-11	1.34E+00
Kd_{sw} (L/Kg)	Kd_{sw} value was calculated by using the correlation equation with K_{oc} that is cited in U.S. EPA (1993d) for an assumed organic carbon fraction of 0.075 in suspended sediment. Measured organic carbon in suspended sediment, specific to site conditions, should be used to calculate Kd_{sw}, because the value varies, depending on the fraction of organic carbon in suspended sediment. Recommended Kd_{sw} value was calculated by using the K_{oc} value that is provided in this table.	B-4-16; B-4-18; B-4-24	1.00E+01
Kd_{bs} (cm^3/g)	Kd_{bs} value was calculated by using the correlation equation with K_{oc} that is cited in U.S. EPA (1993d) for an assumed organic carbon of 0.04 in bottom sediment. Measured organic carbon in bottom sediment, specific to site conditions, should be used to calculate Kd_{bs}, because the value varies depending on the fraction of organic fraction in bottom sediment. Recommended Kd_{bs} value was calculated by using the K_{oc} value that is provided in this table.	B-4-16; B-4-25	5.34E+00

TABLE A-3-192

CHEMICAL-SPECIFIC INPUTS FOR TRICHLOROFLUOROMETHANE (75-69-4)

Parameter	Reference and Explanation	Equations	Value
Chemical/Physical Properties (Continued)			
ksg $(year)^{-1}$	*Ksg* value was calculated by using the chemical half-life in soil, as cited in Howard, Boethling, Jarvis, Meylan, and Michalenko (1991).	B-1-2; B-2-2; B-3-2; B-4-2	7.03E-01
Fv (unitless)	*Fv* value was calculated by using the equation cited in Junge (1977). Recommended value of *Fv* was calculated by using the *Vp* value that is provided in this table.	B-1-1; B-2-1; B-2-7; B-2-8; B-3-1; B-3-7; B-3-8; B-4-1; B-4-8; B-4-9; B-4-12; B-5-1	1.0
Biotransfer Factors for Plants			
RCF $(\frac{\mu g/g\ DW\ plant}{\mu g/mL\ soil\ water})$	*RCF* value was calculated by using the correlation equation with K_{ow} that is cited in Briggs (1982). Recommended value was calculated by using the K_{ow} value that is provided in this table. The value was converted to a dry weight basis by using a moisture content of 87 percent.	B-2-10	2.70E+01
$Br_{root\ veg}$ $(\frac{\mu g/g\ DW\ plant}{\mu g/g\ soil})$	$Br_{root\ veg}$ value was calculated by dividing the *RCF* value with the Kd_s value provided in this table (see section A3.4.2 of Appendix A-3).	B-2-10	2.02E+00
Br_{ag} $(\frac{\mu g/g\ DW\ plant}{\mu g/g\ soil})$	Br_{ag} value was calculated by using the correlation equation with K_{ow} that is cited in Travis and Arms (1988). No distinction was made between values for aboveground produce and forage. Recommended value was calculated by using the K_{ow} value that is provided in this table.	B-2-9	1.33E+00
Br_{forage} $(\frac{\mu g/g\ DW\ plant}{\mu g/g\ soil})$	Br_{forage} value was calculated by using the correlation equation with K_{ow} that is cited in Travis and Arms (1988). No distinction was made between values for aboveground produce and forage. Recommended value was calculated by using the K_{ow} value that is provided in this table.	B-3-9	1.33E+00
Bv_{ag} $(\frac{\mu g/g\ DW\ plant}{\mu g/g\ air})$	Bv_{ag} value was calculated by using the correlation equation with K_{ow} and *H* that is cited in Bacci, Calamari, Gaggi, and Vighi (1990); and Bacci, Cerejeira, Gaggi, Chemello, Calamari, and Vighi (1992); then reducing this value by a factor of 100, as recommended by U.S. EPA (1993d). No distinction was made between values for aboveground produce and forage. Recommended value was calculated, for a temperature (T) of 25°C, by using the *H* and K_{ow} values that are provided in this table.	B-2-8	2.02E-04
Bv_{forage} $(\frac{\mu g/g\ DW\ plant}{\mu g/g\ air})$	Bv_{forage} value was calculated by using the correlation equation with K_{ow} and *H* that is cited in Bacci, Calamari, Gaggi, and Vighi (1990); and Bacci, Cerejeira, Gaggi, Chemello, Calamari, and Vighi (1992); then reducing this value by a factor of 100, as recommended by U.S. EPA (1993d). No distinction was made between values for aboveground produce and forage. Recommended value was calculated, for a temperature (T) of 25°C, by using the *H* and K_{ow} values that are provided in this table.	B-3-8	2.02E-04
Biotransfer Factors for Animals			
Ba_{milk} (day/kg FW)	Ba_{milk} value was calculated by using the correlation equation with K_{ow} that is cited in Travis and Arms (1988). Recommended value was calculated by using the K_{ow} value that is provided in this table.	B-3-11	2.70E-06

TABLE A-3-192

CHEMICAL-SPECIFIC INPUTS FOR TRICHLOROFLUOROMETHANE (75-69-4)

Parameter	Reference and Explanation	Equations	Value
Ba_{beef} (day/kg FW)	Ba_{beef} value was calculated by using the correlation equation with K_{ow} that is cited in Travis and Arms (1988). Recommended value was calculated by using the K_{ow} value that is provided in this table.	B-3-10	8.54E-06
Ba_{pork} (day/kg FW)	Ba_{pork} value was calculated by using thethe fat content ratio of pork to beef (23/19) and multiplying it with the Ba_{beef} value (see section A3.4.2 of Appendix A-3).	B-3-12	1.03E-05
Ba_{eggs} (day/kg FW)	Ba_{eggs} value was calculated by using the correlation equation with K_{ow} that is cited in California EPA (1993). Recommended value was calculated by using the K_{ow} value that is provided in this table.	B-3-13	2.70E-03
$Ba_{chicken}$ (day/kg FW)	$Ba_{chicken}$ value was calculated by using the fat content ratio of chicken to beef (15/19) and multiplying it with the Ba_{beef} value (see section A3.4.3 of Appendix A-3).	B-3-14	6.74E-06
BCF_{fish} (L/kg, FW tissue)	*BCFs* were used for compounds with a log K_{ow} value below 4.0, as cited in U.S. EPA (1995b). BCF_{fish} value calculated using the correlation equation with K_{ow} obtained from Veith, Macek, Petrocelli, and Caroll (1980)—See Appendix A-3.	B-4-26	4.94E+01
BAF_{fish} (L/kg FW)	--	B-4-27	NA
$BSAF_{fish}$ (unitless)	--	B-4-28	NA
Health Benchmarks			
RfD (mg/kg/day)	U.S. EPA (1997b)	C-1-8	3.0E-01
Oral CSF $(mg/kg/day)^{-1}$	--	C-1-7	ND
RfC (mg/m^3)	U.S. EPA (1997c)	C-2-3	7.0E-01
Inhalation URF $(\mu g/m^3)^{-1}$	--	C-2-1	ND
Inhalation CSF $(mg/kg/day)^{-1}$	--	C-2-2	ND

Note:

NA = Not applicable
ND = No data available

All parameters are defined in list of FATE AND TRANSPORT PARAMETERS on page A-3-iii.

TABLE A-3-193

CHEMICAL-SPECIFIC INPUTS FOR 2,4,5-TRICHLOROPHENOL (95-95-4)

Parameter	Reference and Explanation	Equations	Value
Chemical/Physical Properties			
MW (g/mole)	Budavari, O'Neill, Smith, and Heckelman (1989)	--	197.46
T_m (K)	Budavari, O'Neill, Smith, and Heckelman (1989)	--	340.1
Vp (atm)	Geometric mean value cited in U.S. EPA (1994c).	--	2.15E-05 at 25°C (solid)
S (mg/L)	Geometric mean value cited in U.S. EPA (1994c).	--	7.53E+02
H (atm·m^3/mol)	*H* value was calculated by using the theoretical equation from Lyman, Reehl, and Rosenblatt (1982), which defines the constant. Recommended value was calculated by using the *MW*, *S*, and *Vp* values that are provided in this table.	B-1-6; B-2-6; B-2-8; B-3-6; B-4-6; B-4-12; B-4-19	5.64E-06
D_a (cm^2/s)	D_a value was obtained from CHEMDAT8 database (U.S. EPA 1994d).	B-1-6; B-2-6; B-3-6; B-4-6; B-4-21	2.91E-02
D_w (cm^2/s)	D_w value was obtained from CHEMDAT8 database (U.S. EPA 1994d).	B-4-20	7.03E-06
K_{ow} (unitless)	Geometric mean value cited in U.S. EPA (1994c).	--	7.41E+03
K_{oc} (mL/g)	For all ionizing organics, K_{oc} values were estimated on the basis of pH. Estimated values were obtained from U.S. EPA (1994c).	--	pH / K_{oc} 1 2,380 2 2,380 3 2,380 4 2,377 5 2,353 6 2,139 7 1,127 8 223.7 9 56.14 10 37.94 11 36.10 12 35.92 13 35.90 14 35.90
Kd_s (cm^3/g)	Kd_s value was calculated by using the correlation equation with K_{oc} that is cited in U.S. EPA (1993d) for an assumed fraction organic carbon of 0.01 in soil. Measured organic carbon in soil, specific to site conditions, should be used to calculate Kd_s, because the value varies, depending on the fraction of organic carbon in soil. Recommended Kd_s value was calculated by using the K_{oc} value that is provided in this table for a pH of 7.0.	B-1-3; B-1-4; B-1-5; B-1-6; B-2-3; B-2-4; B-2-5; B-2-6; B-2-10; B-3-3; B-3-4; B-3-5; B-3-6; B-4-3; B-4-4; B-4-5; B-4-6; B-4-10; B-4-11	1.13E+01
Kd_{sw} (L/Kg)	Kd_{sw} value was calculated by using the correlation equation with K_{oc} that is cited in U.S. EPA (1993d) for an assumed organic carbon fraction of 0.075 in suspended sediment. Measured organic carbon in suspended sediment, specific to site conditions, should be used to calculate Kd_{sw}, because the value varies, depending on the fraction of organic carbon in suspended sediment. Recommended Kd_{sw} value was calculated by using the K_{oc} value that is provided in this table for a pH of 7.0.	B-4-16; B-4-18; B-4-24	8.45E+01

TABLE A-3-193

CHEMICAL-SPECIFIC INPUTS FOR 2,4,5-TRICHLOROPHENOL (95-95-4)

Parameter	Reference and Explanation	Equations	Value
Chemical/Physical Properties (Continued)			
Kd_{bs} (cm^3/g)	Kd_{bs} value was calculated by using the correlation equation with K_{oc} that is cited in U.S. EPA (1993d) for an assumed organic carbon of 0.04 in bottom sediment. Measured organic carbon in bottom sediment, specific to site conditions, should be used to calculate Kd_{bs}, because the value varies depending on the fraction of organic fraction in bottom sediment. Recommended Kd_{bs} value was calculated by using the K_{oc} value that is provided in this table for a pH of 7.0.	B-4-16; B-4-25	4.51E+01
ksg $(year)^{-1}$	*ksg* value was calculated by using the chemical half-life in soil, as cited in Howard, Boethling, Jarvis, Meylan, and Michalenko (1991).	B-1-2; B-2-2; B-3-2; B-4-2	0.367
Fv (unitless)	*Fv* value was calculated by using equations cited in Junge (1977) and Bidleman (1988). Recommended value of *Fv* was calculated by using *S*, T_m, and *Vp* values that are provided in this table. *Vp* value for this compound was converted to a liquid-phase value before being used in the calculations.	B-1-1; B-2-1; B-2-7; B-2-8; B-3-1; B-3-7; B-3-8; B-4-1; B-4-8; B-4-9; B-4-12; B-5-1	1.0
Biotransfer Factors for Plants			
RCF $(\frac{\mu g/g\ DW\ plant}{\mu g/mL\ soil\ water})$	*RCF* value was calculated by using the correlation equation with K_{ow} that is cited in Briggs (1982). Recommended value was calculated by using the K_{ow} value that is provided in this table. The value was converted to a dry weight basis by using a moisture content of 87 percent.	B-2-10	2.28E+02
$Br_{root\ veg}$ $(\frac{\mu g/g\ DW\ plant}{\mu g/g\ soil})$	$Br_{root\ veg}$ value was calculated by dividing the *RCF* value with the Kd_s value provided in this table.	B-2-10	2.02E+01
Br_{ag} $(\frac{\mu g/g\ DW\ plant}{\mu g/g\ soil})$	Br_{ag} value was calculated by using the correlation equation with K_{ow} that is cited in Travis and Arms (1988). No distinction was made between values for aboveground produce and forage. Recommended value was calculated by using the K_{ow} value that is provided in this table.	B-2-9	2.24E-01
Br_{forage} $(\frac{\mu g/g\ DW\ plant}{\mu g/g\ soil})$	Br_{forage} value was calculated by using the correlation equation with K_{ow} that is cited in Travis and Arms (1988). No distinction was made between values for aboveground produce and forage. Recommended value was calculated by using the K_{ow} value that is provided in this table.	B-3-9	2.24E-01
Bv_{ag} $(\frac{\mu g/g\ DW\ plant}{\mu g/g\ air})$	Bv_{ag} value was calculated by using the correlation equation with K_{ow} and *H* that is cited in Bacci, Calamari, Gaggi, and Vighi (1990); and Bacci, Cerejeira, Gaggi, Chemello, Calamari, and Vighi (1992); then reducing this value by a factor of 100, as recommended by U.S. EPA (1993d). No distinction was made between values for aboveground produce and forage. Recommended value was calculated, for a temperature (T) of 25°C, by using the *H* and K_{ow} values that are provided in this table.	B-2-8	1.31E+02
Bv_{forage} $(\frac{\mu g/g\ DW\ plant}{\mu g/g\ air})$	Bv_{forage} value was calculated by using the correlation equation with K_{ow} and *H* that is cited in Bacci, Calamari, Gaggi, and Vighi (1990); and Bacci, Cerejeira, Gaggi, Chemello, Calamari, and Vighi (1992); then reducing this value by a factor of 100, as recommended by U.S. EPA (1993d). No distinction was made between values for aboveground produce and forage. Recommended value was calculated, for a temperature (T) of 25°C, by using the *H* and K_{ow} values that are provided in this table.	B-3-8	1.31E+02

TABLE A-3-193

CHEMICAL-SPECIFIC INPUTS FOR 2,4,5-TRICHLOROPHENOL (95-95-4)

Parameter	Reference and Explanation	Equations	Value
Biotransfer Factors for Animals			
Ba_{milk} (day/kg FW)	Ba_{milk} value was calculated by using the correlation equation with K_{ow} that is cited in Travis and Arms (1988). Recommended value was calculated by using the K_{ow} value that is provided in this table.	B-3-11	5.89E-05
Ba_{beef} (day/kg FW)	Ba_{beef} value was calculated by using the correlation equation with K_{ow} that is cited in Travis and Arms (1988). Recommended value was calculated by using the K_{ow} value that is provided in this table.	B-3-10	1.86E-04
Ba_{pork} (day/kg FW)	Ba_{pork} value was calculated by using the fat content ratio of pork to beef (23/19) and multiplying it with the Ba_{beef} value.	B-3-12	2.25E-04
Ba_{egg} (day/kg FW)	Ba_{egg} value was calculated by using the correlation equation with K_{ow} that is cited in California EPA (1993). Recommended value was calculated by using the K_{ow} value that is provided in this table.	B-3-13	5.89E-02
$Ba_{chicken}$ (day/kg FW)	$Ba_{chicken}$ value was calculated by using the fat content ratio of chicken to beef (15/19) and multiplying it with the Ba_{beef} value.	B-3-14	1.47E-04
BCF_{fish} (L/kg FW tissue)	*BCFs* were used for compounds with a log K_{ow} value below 4.0, as cited in U.S. EPA (1995b). BCF_{fish} value calculated using the correlation equation with K_{ow} obtained from Veith, Macek, Petrocelli, and Caroll (1980)—See Appendix A-3.	B-4-26	5.14E+02
BAF_{fish} (L/kg FW)	--	B-4-27	NA
$BSAF_{fish}$ (unitless)	--	B-4-28	NA
Health Benchmarks			
RfD (mg/kg/day)	U.S. EPA (1997b)	C-1-8	1.0E-01
Oral CSF $(mg/kg/day)^{-1}$	--	C-1-7	ND
RfC (mg/m^3)	Calculated from *RfD* using an inhalation rate of 20 m^3/day and a human body weight of 70 kg.	C-2-3	3.5E-01
Inhalation URF $(\mu g/m^3)^{-1}$	--	C-2-1	ND
Inhalation CSF $(mg/kg/day)^{-1}$	--	C-2-2	ND

Note:

NA= Not applicable
ND= No data available

All parameters are defined in list of FATE AND TRANSPORT PARAMETERS on page A-3-iii.

TABLE A-3-194

CHEMICAL-SPECIFIC INPUTS FOR 2,4,6-TRICHLOROPHENOL (88-06-2)

Parameter	Reference and Explanation	Equations	Value
Chemical/Physical Properties			
MW (g/mole)	Budavari, O'Neil, Smith, and Heckelman (1989)	--	197.46
T_m (K)	Budavari, O'Neil, Smith, and Heckelman (1989)	--	342.1
Vp (atm)	Geometric mean value cited in U.S. EPA (1994c).	--	1.55E-05 at 25°C (solid)
S (mg/L)	Geometric mean value cited in U.S. EPA (1994c).	--	7.53E+02
H (atm·m^3/mol)	*H* value was calculated by using the theoretical equation from Lyman, Reehl, and Rosenblatt (1982), which defines the constant. Recommended value was calculated by using the *MW*, *S*, and *Vp* values that are provided in this table.	B-1-6; B-2-6; B-2-8; B-3-6; B-4-6; B-4-12; B-4-19	4.06E-06
D_a (cm^2/s)	D_a value was obtained from CHEMDAT8 database (U.S. EPA 1994d).	B-1-6; B-2-6; B-3-6; B-4-6; B-4-21	2.62E-02
D_w (cm^2/s)	D_w value was obtained from CHEMDAT8 database (U.S. EPA 1994d).	B-4-20	8.08E-06
K_{ow} (unitless)	Geometric mean value cited in U.S. EPA (1994c).	--	5.15E+03
K_{oc} (mL/g)	For all ionizing organics, K_{oc} values were estimated on the basis of pH. Estimated values were obtained from U.S. EPA (1994c).	--	pH / K_{oc} 1 1,070 2 1,070 3 1,069 4 1,063 5 1,006 6 670.8 7 226.2 8 120.4 9 108.4 10 107.1 11 107.0 12 107.0 13 107.0 14 107.0
Kd_s (cm^3/g)	Kd_s value was calculated by using the correlation equation with K_{oc} that is cited in U.S. EPA (1993d) for an assumed fraction organic carbon of 0.01 in soil. Measured organic carbon in soil, specific to site conditions, should be used to calculate Kd_s, because the value varies, depending on the fraction of organic carbon in soil. Recommended Kd_s value was calculated by using the K_{oc} value that is provided in this table for a pH of 7.0.	B-1-3; B-1-4; B-1-5; B-1-6; B-2-3; B-2-4; B-2-5; B-2-6; B-2-10; B-3-3; B-3-4; B-3-5; B-3-6; B-4-3; B-4-4; B-4-5; B-4-6; B-4-10; B-4-11	2.26E+00

TABLE A-3-194

CHEMICAL-SPECIFIC INPUTS FOR 2,4,6-TRICHLOROPHENOL (88-06-2)

Parameter	Reference and Explanation	Equations	Value
Chemical/Physical Properties (Continued)			
Kd_{sw} (L/Kg)	Kd_{sw} value was calculated by using the correlation equation with K_{oc} that is cited in U.S. EPA (1993d) for an assumed organic carbon fraction of 0.075 in suspended sediment. Measured organic carbon in suspended sediment, specific to site conditions, should be used to calculate Kd_{sw}, because the value varies, depending on the fraction of organic carbon in suspended sediment. Recommended Kd_{sw} value was calculated by using the K_{oc} value that is provided in this table for a pH of 7.0.	B-4-16; B-4-18; B-4-24	1.70E+01
Kd_{bs} (cm^3/g)	Kd_{bs} value was calculated by using the correlation equation with K_{oc} that is cited in U.S. EPA (1993d) for an assumed organic carbon of 0.04 in bottom sediment. Measured organic carbon in bottom sediment, specific to site conditions, should be used to calculate Kd_{bs}, because the value varies depending on the fraction of organic fraction in bottom sediment. Recommended Kd_{bs} value was calculated by using the K_{oc} value that is provided in this table for a pH of 7.0.	B-4-16; B-4-25	9.05E+00
ksg $(year)^{-1}$	*Ksg* value was calculated by using the chemical half-life in soil, as cited in Howard, Boethling, Jarvis, Meylan, and Michalenko (1991).	B-1-1; B-1-2; B-2-1; B-2-2; B-3-1; B-3-2; B-4-1; B-4-2	3.61E+00
Fv (unitless)	*Fv* value was calculated by using equations cited in Junge (1977) and Bidleman (1988). Recommended value of *Fv* was calculated by using *S*, T_m, and *Vp* values that are provided in this table. *Vp* value for this compound was converted to a liquid-phase value before being used in the calculations.	B-1-1; B-2-1; B-2-7; B-2-8; B-3-1; B-3-7; B-3-8; B-4-1; B-4-8; B-4-9; B-4-12; B-5-1	1.0
Biotransfer Factors for Plants			
RCF $(\frac{\mu g/g\ DW\ plant}{\mu g/mL\ soil\ water})$	*RCF* value was calculated by using the correlation equation with K_{ow} that is cited in Briggs (1982). Recommended value was calculated by using the K_{ow} value that is provided in this table. The value was converted to a dry weight basis by using a moisture content of 87 percent.	B-2-10	1.74E+02
$Br_{root\ veg}$ $(\frac{\mu g/g\ DW\ plant}{\mu g/g\ soil})$	$Br_{root\ veg}$ value was calculated by dividing the *RCF* value with the Kd_s value provided in this table.	B-2-10	7.69E+01
Br_{ag} $(\frac{\mu g/g\ DW\ plant}{\mu g/g\ soil})$	Br_{ag} value was calculated by using the correlation equation with K_{ow} that is cited in Travis and Arms (1988). No distinction was made between values for aboveground produce and forage. Recommended value was calculated by using the K_{ow} value that is provided in this table.	B-2-9	2.77E-01
Br_{forage} $(\frac{\mu g/g\ DW\ plant}{\mu g/g\ soil})$	Br_{forage} value was calculated by using the correlation equation with K_{ow} that is cited in Travis and Arms (1988). No distinction was made between values for aboveground produce and forage. Recommended value was calculated by using the K_{ow} value that is provided in this table.	B-3-9	2.77E-01

TABLE A-3-194

CHEMICAL-SPECIFIC INPUTS FOR 2,4,6-TRICHLOROPHENOL (88-06-2)

Parameter	Reference and Explanation	Equations	Value
Biotransfer Factors for Plants (Continued)			
Bv_{ag} ($\frac{\mu g/g\ DW\ plant}{\mu g/g\ air}$)	Bv_{ag} value was calculated by using the correlation equation with K_{ow} and H that is cited in Bacci, Calamari, Gaggi, and Vighi (1990); and Bacci, Cerejeira, Gaggi, Chemello, Calamari, and Vighi (1992); then reducing this value by a factor of 100, as recommended by U.S. EPA (1993d). No distinction was made between values for aboveground produce and forage. Recommended value was calculated, for a temperature (T) of 25°C, by using the H and K_{ow} values that are provided in this table.	B-2-8	1.23E+02
Bv_{forage} ($\frac{\mu g/g\ DW\ plant}{\mu g/g\ air}$)	Bv_{forage} value was calculated by using the correlation equation with K_{ow} and H that is cited in Bacci, Calamari, Gaggi, and Vighi (1990); and Bacci, Cerejeira, Gaggi, Chemello, Calamari, and Vighi (1992); then reducing this value by a factor of 100, as recommended by U.S. EPA (1993d). No distinction was made between values for aboveground produce and forage. Recommended value was calculated, for a temperature (T) of 25°C, by using the H and K_{ow} values that are provided in this table.	B-3-8	1.23E+02
Biotransfer Factors for Animals			
Ba_{milk} (day/kg FW)	Ba_{milk} value was calculated by using the correlation equation with K_{ow} that is cited in Travis and Arms (1988). Recommended value was calculated by using the K_{ow} value that is provided in this table.	B-3-11	4.09E-05
Ba_{beef} (day/kg FW)	Ba_{beef} value was calculated by using the correlation equation with K_{ow} that is cited in Travis and Arms (1988). Recommended value was calculated by using the K_{ow} value that is provided in this table.	B-3-10	1.29E-04
Ba_{pork} (day/kg FW)	Ba_{pork} value was calculated by using thethe fat content ratio of pork to beef (23/19) and multiplying it with the Ba_{beef} value.	B-3-12	1.57E-04
Ba_{eggs} (day/kg FW)	Ba_{eggs} value was calculated by using the correlation equation with K_{ow} that is cited in California EPA (1993). Recommended value was calculated by using the K_{ow} value that is provided in this table.	B-3-13	4.09E-02
$Ba_{chicken}$ (day/kg FW)	$Ba_{chicken}$ value was calculated by using the fat content ratio of chicken to beef (15/19) and multiplying it with the Ba_{beef} value.	B-3-14	1.02E-04
BCF_{fish} (L/kg, FW tissue)	*BCFs* were used for compounds with a log K_{ow} value below 4.0, as cited in U.S. EPA (1995b). BCF_{fish} value calculated using the correlation equation with K_{ow} obtained from Veith, Macek, Petrocelli, and Caroll (1980)—See Appendix A-3.	B-4-26	3.90E+02
BAF_{fish} (L/kg FW)	--	B-4-27	NA
$BSAF_{fish}$ (unitless)	--	B-4-28	NA
Health Benchmarks			
RfD (mg/kg/day)	--	C-1-8	--
Oral CSF $(mg/kg/day)^{-1}$	U.S. EPA (1995b)	C-1-7	1.1E-02
RfC (mg/m^3)	--	C-2-3	--
Inhalation URF $(\mu g/m^3)^{-1}$	U.S. EPA (1997)	C-2-1	3.1E-06
Inhalation CSF $(mg/kg/day)^{-1}$	--	C-2-2	--

TABLE A-3-194

CHEMICAL-SPECIFIC INPUTS FOR 2,4,6-TRICHLOROPHENOL (88-06-2)

Note:

NA = Not applicable
ND = No data available

All parameters are defined in list of FATE AND TRANSPORT PARAMETERS on page A-3-iii.

TABLE A-3-195

CHEMICAL-SPECIFIC INPUTS FOR 1,2,3-TRICHLOROPROPANE (96-18-4)

Parameter	Reference and Explanation	Equations	Value
Chemical/Physical Properties			
MW (g/mole)	Montgomery and Welkom (1991)	--	147.43
T_m (K)	Montgomery and Welkom (1991)	--	258.4
Vp (atm)	*Vp* value cited in U.S. EPA (1995b).	--	4.90E-03 at 25°C (liquid)
S (mg/L)	*S* value cited in U.S. EPA (1995b).	--	1.90E+03
H (atm·m^3/mol)	*H* value was calculated by using the theoretical equation from Lyman, Reehl, and Rosenblatt (1982), which defines the constant. Recommended value was calculated by using the *MW*, *S*, and *Vp* values that are provided in this table.	B-1-6; B-2-6; B-2-8; B-3-6; B-4-6; B-4-12; B-4-19	3.80E-04
D_a (cm^2/s)	D_a value was obtained from CHEMDAT8 database (U.S. EPA 1994d).	B-1-6; B-2-6; B-3-6; B-4-6; B-4-21	3.99E-02
D_w (cm^2/s)	D_w value was obtained from CHEMDAT8 database (U.S. EPA 1994d).	B-4-20	9.24E-06
K_{ow} (unitless)	Arithmetic mean value cited in Karickhoff and Long (1995).	--	1.78E+02
K_{oc} (mL/g)	K_{oc} value was calculated by using the correlation equation with K_{ow} for all nonionizing organics except phthalates, PAHs, dioxins, and furans as cited in U.S. EPA (1994c). K_{oc} value was calculated by using the recommended K_{ow} value that is provided in this table.	--	8.05E+01
Kd_s (cm^3/g)	Kd_s value was calculated by using the correlation equation with K_{oc} that is cited in U.S. EPA (1993d) for an assumed fraction organic carbon of 0.01 in soil. Measured organic carbon in soil, specific to site conditions, should be used to calculate Kd_s, because the value varies, depending on the fraction of organic carbon in soil. Recommended Kd_s value was calculated by using the K_{oc} value that is provided in this table.	B-1-3; B-1-4; B-1-5; B-1-6; B-2-3; B-2-4; B-2-5; B-2-6; B-2-10; B-3-3; B-3-4; B-3-5; B-3-6; B-4-3; B-4-4; B-4-5; B-4-6; B-4-10; B-4-11	8.10E-01
Kd_{sw} (L/Kg)	Kd_{sw} value was calculated by using the correlation equation with K_{oc} that is cited in U.S. EPA (1993d) for an assumed organic carbon fraction of 0.075 in suspended sediment. Measured organic carbon in suspended sediment, specific to site conditions, should be used to calculate Kd_{sw}, because the value varies, depending on the fraction of organic carbon in suspended sediment. Recommended Kd_{sw} value was calculated by using the K_{oc} value that is provided in this table.	B-4-16; B-4-18; B-4-24	6.04E+00
Kd_{bs} (cm^3/g)	Kd_{bs} value was calculated by using the correlation equation with K_{oc} that is cited in U.S. EPA (1993d) for an assumed organic carbon of 0.04 in bottom sediment. Measured organic carbon in bottom sediment, specific to site conditions, should be used to calculate Kd_{bs}, because the value varies depending on the fraction of organic fraction in bottom sediment. Recommended Kd_{bs} value was calculated by using the K_{oc} value that is provided in this table.	B-4-16; B-4-25	3.22E+00

TABLE A-3-195

CHEMICAL-SPECIFIC INPUTS FOR 1,2,3-TRICHLOROPROPANE (96-18-4)

Parameter	Reference and Explanation	Equations	Value
Chemical/Physical Properties (Continued)			
ksg $(year)^{-1}$	*ksg* value was calculated by using the chemical half-life in soil, as cited in Howard, Boethling, Jarvis, Meylan, and Michalenko (1991).	B-1-2; B-2-2; B-3-2; B-4-2	7.03E-01
Fv (unitless)	*Fv* value was calculated by using the equation cited in Junge (1977). Recommended value of *Fv* was calculated by using the *Vp* value that is provided in this table.	B-1-1; B-2-1; B-2-7; B-2-8; B-3-1; B-3-7; B-3-8; B-4-1; B-4-8; B-4-9; B-4-12; B-5-1	1.0
Biotransfer Factors for Plants			
RCF $(\frac{\mu g/g\ DW\ plant}{\mu g/mL\ soil\ water})$	*RCF* value was calculated by using the correlation equation with K_{ow} that is cited in Briggs (1982). Recommended value was calculated by using the K_{ow} value that is provided in this table. The value was converted to a dry weight basis by using a moisture content of 87 percent.	B-2-10	1.89E+01
$Br_{root\ veg}$ $(\frac{\mu g/g\ DW\ plant}{\mu g/g\ soil})$	$Br_{root\ veg}$ value was calculated by dividing the *RCF* value with the Kd_s value provided in this table.	B-2-10	2.34E+01
Br_{ag} $(\frac{\mu g/g\ DW\ plant}{\mu g/g\ soil})$	Br_{ag} value was calculated by using the correlation equation with K_{ow} that is cited in Travis and Arms (1988). No distinction was made between values for aboveground produce and forage. Recommended value was calculated by using the K_{ow} value that is provided in this table.	B-2-9	1.94E+00
Br_{forage} $(\frac{\mu g/g\ DW\ plant}{\mu g/g\ soil})$	Br_{forage} value was calculated by using the correlation equation with K_{ow} that is cited in Travis and Arms (1988). No distinction was made between values for aboveground produce and forage. Recommended value was calculated by using the K_{ow} value that is provided in this table.	B-3-9	1.94E+00
Bv_{ag} $(\frac{\mu g/g\ DW\ plant}{\mu g/g\ air})$	Bv_{ag} value was calculated by using the correlation equation with K_{ow} and *H* that is cited in Bacci, Calamari, Gaggi, and Vighi (1990); and Bacci, Cerejeira, Gaggi, Chemello, Calamari, and Vighi (1992); then reducing this value by a factor of 100, as recommended by U.S. EPA (1993d). No distinction was made between values for aboveground produce and forage. Recommended value was calculated, for a temperature (T) of 25°C, by using the *H* and K_{ow} values that are provided in this table.	B-2-8	3.66E-02
Bv_{forage} $(\frac{\mu g/g\ DW\ plant}{\mu g/g\ air})$	Bv_{forage} value was calculated by using the correlation equation with K_{ow} and *H* that is cited in Bacci, Calamari, Gaggi, and Vighi (1990); and Bacci, Cerejeira, Gaggi, Chemello, Calamari, and Vighi (1992); then reducing this value by a factor of 100, as recommended by U.S. EPA (1993d). No distinction was made between values for aboveground produce and forage. Recommended value was calculated, for a temperature (T) of 25°C, by using the *H* and K_{ow} values that are provided in this table.	B-3-8	3.66E-02
Biotransfer Factors for Animals			
Ba_{milk} (day/kg FW)	Ba_{milk} value was calculated by using the correlation equation with K_{ow} that is cited in Travis and Arms (1988). Recommended value was calculated by using the K_{ow} value that is provided in this table.	B-3-11	1.41E-06
Ba_{beef} (day/kg FW	Ba_{beef} value was calculated by using the correlation equation with K_{ow} that is cited in Travis and Arms (1988). Recommended value was calculated by using the K_{ow} value that is provided in this table.	B-3-10	4.47E-06

TABLE A-3-195

CHEMICAL-SPECIFIC INPUTS FOR 1,2,3-TRICHLOROPROPANE (96-18-4)

Parameter	Reference and Explanation	Equations	Value
Ba_{pork} (day/kg FW	Ba_{pork} value was calculated by using the fat content ratio of pork to beef (23/19) and multiplying it with the Ba_{beef} value.	B-3-12	5.41E-06
Ba_{egg} (day/kg FW)	Ba_{egg} value was calculated by using the correlation equation with K_{ow} that is cited in California EPA (1993). Recommended value was calculated by using the K_{ow} value that is provided in this table.	B-3-13	1.41E-03
$Ba_{chicken}$ (day/kg FW)	$Ba_{chicken}$ value was calculated by using the fat content ratio of chicken to beef (15/19) and multiplying it with the Ba_{beef} value.	B-3-14	3.53E-06
BCF_{fish} (L/kg FW tissue)	*BCFs* were used for compounds with a log K_{ow} value below 4.0, as cited in U.S. EPA (1995b). BCF_{fish} value calculated using the correlation equation with K_{ow} obtained from Veith, Macek, Petrocelli, and Caroll (1980)—See Appendix A-3.	B-4-26	3.02E+01
BAF_{fish} (L/kg FW	--	B-4-27	NA
$BSAF_{fish}$ (unitless)	--	B-4-28	NA
Health Benchmarks			
RfD (mg/kg/day)	U.S. EPA (1997b)	C-1-8	6.0E-03
Oral CSF $(mg/kg/day)^{-1}$	U.S. EPA (1997c)	C-1-7	7.0E+00
RfC (mg/m^3)	Calculated from *RfD* using an inhalation rate of 20 m^3/day and a human body weight of 70 kg.	C-2-3	2.1E-02
Inhalation URF $(\mu g/m^3)^{-1}$	Calculated from *Oral CSF* using an inhalation rate of 20 m^3/day and a human body weight of 70 kg.	C-2-1	2.0E-03
Inhalation CSF $(mg/kg/day)^{-1}$	Value based on *Oral CSF* assuming route-to-route extrapolation.	C-2-2	7.0E+00

Note:

NA= Not applicable
ND= No data available

All parameters are defined in list of FATE AND TRANSPORT PARAMETERS on page A-3-iii.

TABLE A-3-196

CHEMICAL-SPECIFIC INPUTS FOR 1,3,5-TRIMETHYLBENZENE (108-67-8)

Parameter	Reference and Explanation	Equations	Value
Chemical/Physical Properties			
MW (g/mole)	Budavari, O'Neil, Smith, and Heckelman (1989)	--	120.19
T_m (K)	Montgomery and Welkom (1991)	--	287.9
Vp (atm)	*Vp* value cited in U.S. EPA (1992a).	--	1.30E-03 at 25°C (liquid)
S (mg/L)	*S* value cited in U.S. EPA (1992a).	--	2.00E+01
H (atm·m^3/mol)	*H* value was calculated by using the theoretical equation from Lyman, Reehl, and Rosenblatt (1982), which defines the constant. Recommended value was calculated by using the *MW*, *S*, and *Vp* values that are provided in this table.	B-1-6; B-2-6; B-2-8; B-3-6; B-4-6; B-4-12; B-4-19	7.81E-03
D_a (cm^2/s)	D_a value was obtained from CHEMDAT8 database (U.S. EPA 1994d).	B-1-6; B-2-6; B-3-6; B-4-6; B-4-21	6.48E-02
D_w (cm^2/s)	D_w value was obtained from CHEMDAT8 database (U.S. EPA 1994d).	B-4-20	7.86E-06
K_{ow} (unitless)	K_{ow} value cited in Howard (1989-1993).	--	2.63E+03
K_{oc} (mL/g)	K_{oc} value was calculated by using the correlation equation with K_{ow} for phthalates and PAHs, / all nonionizing organics except phthalates, PAHs, dioxins, and furans, cited in U.S. EPA (1994c). K_{oc} value was calculated by using the recommended K_{ow} value that is provided in this table.	--	1.67E+03
Kd_s (cm^3/g)	Kd_s value was calculated by using the correlation equation with K_{oc} that is cited in U.S. EPA (1993d) for an assumed organic carbon fraction of 0.01 in soil. Measured organic carbon in soil, specific to site conditions, should be used to calculate Kd_s, because the value varies, depending on the fraction of organic carbon in soil. Recommended Kd_s value was calculated by using the K_{oc} value that is provided in this table.	B-1-3; B-1-4; B-1-5; B-1-6; B-2-3; B-2-4; B-2-5; B-2-6; B-2-10; B-3-3; B-3-4; B-3-5; B-3-6; B-4-3; B-4-4; B-4-5; B-4-6; B-4-10; B-4-11	1.67E+01
Kd_{sw} (L/Kg)	Kd_{sw} value was calculated by using the correlation equation with K_{oc} that is cited in U.S. EPA (1993d) for an assumed organic carbon fraction of 0.075 in suspended sediment. Measured organic carbon in suspended sediment, specific to site conditions, should be used to calculate Kd_{sw}, because the value varies, depending on the fraction of organic carbon in suspended sediment. Recommended Kd_{sw} value was calculated by using the K_{oc} value that is provided in this table.	B-4-16; B-4-18; B-4-24	1.25E+02
Chemical/Physical Properties (Continued)			

TABLE A-3-196

CHEMICAL-SPECIFIC INPUTS FOR 1,3,5-TRIMETHYLBENZENE (108-67-8)

Parameter	Reference and Explanation	Equations	Value
Kd_{bs} (cm^3/g)	Kd_{bs} value was calculated by using the correlation equation with K_{oc} that is cited in U.S. EPA (1993d) for an assumed organic carbon fraction of 0.04 in bottom sediment. Measured organic carbon in bottom sediment, specific to site conditions, should be used to calculate Kd_{bs}, because the value varies, depending on the fraction of organic carbon in bottom sediment. Recommended Kd_{bs} value was calculated by using the K_{oc} value that is provided in this table.	B-4-16; B-4-25	6.69E+01
ksg $(year)^{-1}$	*Ksg* value was calculated by using the chemical half-life in soil, as cited in Mackay, Shiu, and Ma (1992).	B-1-2; B-2-2; B-3-2; B-4-2	3.16E+01
Fv (unitless)	*Fv* value was calculated by using the equation cited in Junge (1977). Recommended value of *Fv* was calculated by using the *Vp* value that is provided in the table.	B-1-1; B-2-1; B-2-7; B-2-8; B-3-1; B-3-7; B-3-8; B-4-1; B-4-8; B-4-9; B-4-12; B-5-1	1.00
Biotransfer Factors for Plants			
RCF $(\frac{\mu g/g\ DW\ plant}{\mu g/mL\ soil\ water})$	*RCF* value was calculated by using the correlation equation with K_{ow} that is cited in Briggs (1982). Recommended value was calculated by using the K_{ow} value that is provided in this table. The value was then converted to a dry weight basis by using a moisture content of 87 percent.	B-2-10	1.06E+02
$Br_{root\ veg}$ $(\frac{\mu g/g\ DW\ plant}{\mu g/g\ soil})$	$Br_{root\ veg}$ value was calculated by dividing the *RCF* value with the Kd_s value provided in this table.	B-2-10	6.35E+00
Br_{ag} $(\frac{\mu g/g\ DW\ plant}{\mu g/g\ soil})$	Br_{ag} value was calculated by using the correlation equation with K_{ow} that is cited in Travis and Arms (1988). No distinction was made between values for aboveground produce and forage. Recommended value was calculated by using the K_{ow} value that is provided in this table.	B-2-9	4.09E-01
Br_{forage} $(\frac{\mu g/g\ DW\ plant}{\mu g/g\ soil})$	Br_{forage} value was calculated by using the correlation equation with K_{ow} that is cited in Travis and Arms (1988). No distinction was made between values for aboveground produce and forage. Recommended value was calculated by using the K_{ow} value that is provided in this table.	B-3-9	4.09E-01
Bv_{ag} $(\frac{\mu g/g\ DW\ plant}{\mu g/g\ air})$	Bv_{ag} value was calculated by using the correlation equation with K_{ow} and *H* that is cited in Bacci, Calamari, Gaggi, and Vighi (1990); and Bacci, Cerejeira, Gaggi, Chemello, Calamari, and Vighi (1992); then reducing this value by a factor of 100. No distinction was made between values for aboveground produce and forage. Recommended value was calculated, for a temperature (T) of 25°C, by using the *H* and K_{ow} values that are provided in this table.	B-3-8	3.14E-02
Bv_{forage} $(\frac{\mu g/g\ DW\ plant}{\mu g/g\ air})$	Bv_{forage} value was calculated by using the correlation equation with K_{ow} and *H* that is cited in Bacci, Calamari, Gaggi, and Vighi (1990); and Bacci, Cerejeira, Gaggi, Chemello, Calamari, and Vighi (1992); then reducing this value by a factor of 100. No distinction was made between values for aboveground produce and forage. Recommended value was calculated, for a temperature (T) of 25°C, by using the *H* and K_{ow} values that are provided in this table.	B-3-8	3.14E-02

TABLE A-3-196

CHEMICAL-SPECIFIC INPUTS FOR 1,3,5-TRIMETHYLBENZENE (108-67-8)

Parameter	Reference and Explanation	Equations	Value
Biotransfer Factors for Animals			
Ba_{milk} (day/kg FW)	Ba_{milk} value was calculated by using the correlation equation with K_{ow} that is cited in Travis and Arms (1988). Recommended value was calculated by using the K_{ow} value that is provided in this table.	B-3-11	2.09E-05
Ba_{beef} (day/kg FW)	Ba_{beef} value was calculated by using the correlation equation with K_{ow} that is cited in Travis and Arms (1988). Recommended value was calculated by using the K_{ow} value that is provided in this table.	B-3-10	6.61E-05
Ba_{pork} (day/kg FW)	Ba_{pork} value was calculated by using the fat content ratio of pork to beef (23/19) and multiplying it with the Ba_{beef} value.	B-3-12	8.00E-05
Ba_{egg} (day/kg FW)	Ba_{egg} value was calculated by using the correlation equation with K_{ow} that is cited in California EPA (1993). Recommended value was calculated by using the K_{ow} value that is provided in this table.	B-3-13	2.09E-02
$Ba_{chicken}$ (day/kg FW)	$Ba_{chicken}$ value was calculated by using the fat content ratio of chicken to beef (15/19) and multiplying it with the Ba_{beef} value.	B-3-14	5.22E-05
BCF_{fish} (L/kg FW tissue)	*BCFs* were used for compounds with a log K_{ow} value below 4.0, as cited in U.S. EPA (1995b). BCF_{fish} value calculated using the correlation equation with K_{ow} obtained from Veith, Macek, Petrocelli, and Caroll (1980)—See Appendix A-3.	B-4-26	2.34E+02
BAF_{fish} (L/kg FW)	--	B-4-27	NA
$BSAF_{fish}$ (unitless)	--	B-4-28	NA
Health Benchmarks			
RfD (mg/kg/day)	U.S. EPA (1997a)	C-1-8	5.0E-02
Oral CSF $(mg/kg/day)^{-1}$		C-1-7	ND
RfC (mg/m^3)	Calculated from *RfD* using an inhalation rate of 20 m^3/day and a human body weight of 70 kg.	C-2-3	1.8E-01
Inhalation URF $(\mu g/m^3)^{-1}$		C-2-1	ND
Inhalation CSF $(mg/kg/day)^{-1}$		C-2-2	ND

Note:

NA = Not applicable
ND = No data available

All parameters are defined in list of FATE AND TRANSPORT PARAMETERS on page A-3-iii.

TABLE A-3-197

CHEMICAL-SPECIFIC INPUTS FOR 1,3,5-TRINITROBENZENE (99-35-4)

Parameter	Reference and Explanation	Equations	Value
Chemical/Physical Properties			
MW (g/mole)	Budavari, O'Neill, Smith, and Heckelman (1989)	--	213.11
T_m (K)	Budavari, O'Neill, Smith, and Heckelman (1989)	--	395.6
Vp (atm)	*Vp* value cited in U.S. EPA (1995b).	--	1.30E-07 at 25°C (solid)
S (mg/L)	*S* value cited in U.S. EPA (1995b).	--	3.20E+02
H (atm·m^3/mol)	*H* value was calculated by using the theoretical equation from Lyman, Reehl, and Rosenblatt (1982), which defines the constant. Recommended value was calculated by using the *MW*, *S*, and *Vp* values that are provided in this table.	B-1-6; B-2-6; B-2-8; B-3-6; B-4-6; B-4-12; B-4-19	8.66E-08
D_a (cm^2/s)	D_a value was obtained from WATER8 model database (U.S. EPA 1995d).	B-1-6; B-2-6; B-3-6; B-4-6; B-4-21	2.84E-02
D_w (cm^2/s)	D_w value was obtained from WATER8 model database (U.S. EPA 1995d).	B-4-20	6.08E-06
K_{ow} (unitless)	Arithmetic mean value cited in Karickhoff and Long (1995).	--	1.51E+01
K_{oc} (mL/g)	K_{oc} value was calculated by using the correlation equation with K_{ow} for all nonionizing organics except phthalates, PAHs, dioxins, and furans as cited in U.S. EPA (1994c). K_{oc} value was calculated by using the recommended K_{ow} value that is provided in this table.	--	1.18E+01
Kd_s (cm^3/g)	Kd_s value was calculated by using the correlation equation with K_{oc} that is cited in U.S. EPA (1993d) for an assumed fraction organic carbon of 0.01 in soil. Measured organic carbon in soil, specific to site conditions, should be used to calculate Kd_s, because the value varies, depending on the fraction of organic carbon in soil. Recommended Kd_s value was calculated by using the K_{oc} value that is provided in this table.	B-1-3; B-1-4; B-1-5; B-1-6; B-2-3; B-2-4; B-2-5; B-2-6; B-2-10; B-3-3; B-3-4; B-3-5; B-3-6; B-4-3; B-4-4; B-4-5; B-4-6; B-4-10; B-4-11	1.18E-01
Kd_{sw} (L/Kg)	Kd_{sw} value was calculated by using the correlation equation with K_{oc} that is cited in U.S. EPA (1993d) for an assumed organic carbon fraction of 0.075 in suspended sediment. Measured organic carbon in suspended sediment, specific to site conditions, should be used to calculate Kd_{sw}, because the value varies, depending on the fraction of organic carbon in suspended sediment. Recommended Kd_{sw} value was calculated by using the K_{oc} value that is provided in this table.	B-4-16; B-4-18; B-4-24	8.84E-01
Kd_{bs} (cm^3/g)	Kd_{bs} value was calculated by using the correlation equation with K_{oc} that is cited in U.S. EPA (1993d) for an assumed organic carbon of 0.04 in bottom sediment. Measured organic carbon in bottom sediment, specific to site conditions, should be used to calculate Kd_{bs}, because the value varies depending on the fraction of organic fraction in bottom sediment. Recommended Kd_{bs} value was calculated by using the K_{oc} value that is provided in this table.	B-4-16; B-4-25	4.72E-01

TABLE A-3-197

CHEMICAL-SPECIFIC INPUTS FOR 1,3,5-TRINITROBENZENE (99-35-4)

Parameter	Reference and Explanation	Equations	Value
Chemical/Physical Properties (Continued)			
ksg $(year)^{-1}$	*Ksg* value was assumed to be 0 due to a lack of data.	B-1-2; B-2-2; B-3-2; B-4-2	0.0
Fv (unitless)	*Fv* value was calculated by using equations cited in Junge (1977) and Bidleman (1988). Recommended value of *Fv* was calculated by using *S*, T_m, and *Vp* values that are provided in this table. *Vp* value for this compound was converted to a liquid-phase value before being used in the calculations.	B-1-1; B-2-1; B-2-7; B-2-8; B-3-1; B-3-7; B-3-8; B-4-1; B-4-8; B-4-9; B-4-12; B-5-1	1.0
Biotransfer Factors for Plants			
RCF $(\frac{\mu g/g\ DW\ plant}{\mu g/mL\ soil\ water})$	*RCF* value was calculated by using the correlation equation with K_{ow} that is cited in Briggs (1982). Recommended value was calculated by using the K_{ow} value that is provided in this table. The value was converted to a dry weight basis by using a moisture content of 87 percent.	B-2-10	8.19E+00
$Br_{root\ veg}$ $(\frac{\mu g/g\ DW\ plant}{\mu g/g\ soil})$	$Br_{root\ veg}$ value was calculated by dividing the *RCF* value with the Kd_s value provided in this table.	B-2-10	6.95E+01
Br_{ag} $(\frac{\mu g/g\ DW\ plant}{\mu g/g\ soil})$	Br_{ag} value was calculated by using the correlation equation with K_{ow} that is cited in Travis and Arms (1988). No distinction was made between values for aboveground produce and forage. Recommended value was calculated by using the K_{ow} value that is provided in this table.	B-2-9	8.05E+00
Br_{forage} $(\frac{\mu g/g\ DW\ plant}{\mu g/g\ soil})$	Br_{forage} value was calculated by using the correlation equation with K_{ow} that is cited in Travis and Arms (1988). No distinction was made between values for aboveground produce and forage. Recommended value was calculated by using the K_{ow} value that is provided in this table.	B-3-9	8.05E+00
Bv_{ag} $(\frac{\mu g/g\ DW\ plant}{\mu g/g\ air})$	Bv_{ag} value was calculated by using the correlation equation with K_{ow} and *H* that is cited in Bacci, Calamari, Gaggi, and Vighi (1990); and Bacci, Cerejeira, Gaggi, Chemello, Calamari, and Vighi (1992); then reducing this value by a factor of 100, as recommended by U.S. EPA (1993d). No distinction was made between values for aboveground produce and forage. Recommended value was calculated, for a temperature (T) of 25ºC, by using the *H* and K_{ow} values that are provided in this table.	B-2-8	1.17E+01
Bv_{forage} $(\frac{\mu g/g\ DW\ plant}{\mu g/g\ air})$	Bv_{forage} value was calculated by using the correlation equation with K_{ow} and *H* that is cited in Bacci, Calamari, Gaggi, and Vighi (1990); and Bacci, Cerejeira, Gaggi, Chemello, Calamari, and Vighi (1992); then reducing this value by a factor of 100, as recommended by U.S. EPA (1993d). No distinction was made between values for aboveground produce and forage. Recommended value was calculated, for a temperature (T) of 25ºC, by using the *H* and K_{ow} values that are provided in this table.	B-3-8	1.17E+01
Biotransfer Factors for Animals			
Ba_{milk} (day/kg FW)	Ba_{milk} value was calculated by using the correlation equation with K_{ow} that is cited in Travis and Arms (1988). Recommended value was calculated by using the K_{ow} value that is provided in this table.	B-3-11	1.20E-07

TABLE A-3-197

CHEMICAL-SPECIFIC INPUTS FOR 1,3,5-TRINITROBENZENE (99-35-4)

Parameter	Reference and Explanation	Equations	Value
Ba_{beef} (day/kg FW)	Ba_{beef} value was calculated by using the correlation equation with K_{ow} that is cited in Travis and Arms (1988). Recommended value was calculated by using the K_{ow} value that is provided in this table.	B-3-10	3.80E-07
Ba_{pork} (day/kg FW)	Ba_{pork} value was calculated by using the fat content ratio of pork to beef (23/19) and multiplying it with the Ba_{beef} value.	B-3-12	4.60E-07
Ba_{egg} (day/kg FW)	Ba_{egg} value was calculated by using the correlation equation with K_{ow} that is cited in California EPA (1993). Recommended value was calculated by using the K_{ow} value that is provided in this table.	B-3-13	1.20E-04
$Ba_{chicken}$ (day/kg FW)	$Ba_{chicken}$ value was calculated by using the fat content ratio of chicken to beef (15/19) and multiplying it with the Ba_{beef} value.	B-3-14	3.00E-07
BCF_{fish} (L/kg FW tissue)	*BCFs* were used for compounds with a log K_{ow} value below 4.0, as cited in U.S. EPA (1995b). BCF_{fish} value calculated using the correlation equation with K_{ow} obtained from Veith, Macek, Petrocelli, and Caroll (1980)—See Appendix A-3.	B-4-26	4.64E+00
BAF_{fish} (L/kg FW)	--	B-4-27	NA
$BSAF_{fish}$ (unitless)	--	B-4-28	NA
Health Benchmarks			
RfD (mg/kg/day)	U.S. EPA (1997b)	C-1-8	3.0E-02
Oral CSF $(mg/kg/day)^{-1}$	--	C-1-7	ND
RfC (mg/m^3)	Calculated from *RfD* using an inhalation rate of 20 m^3/day and a human body weight of 70 kg.	C-2-3	1.1E-01
Inhalation URF $(\mu g/m^3)^{-1}$	--	C-2-1	ND
Inhalation CSF $(mg/kg/day)^{-1}$	--	C-2-2	ND

Note:

NA= Not applicable
ND= No data available

All parameters are defined in list of FATE AND TRANSPORT PARAMETERS on page A-3-iii.

TABLE A-3-198

CHEMICAL-SPECIFIC INPUTS FOR 2,4,6 -TRINITROTOLUENE (118-96-7)

Parameter	Reference and Explanation	Equations	Value
Chemical/Physical Properties			
MW (g/mole)	Budavari, O'Neil, Smith, and Heckelman (1989)	--	227.13
T_m (K)	Montgomery and Welkom (1991)	--	353.2
Vp (atm)	--	--	ND
S (mg/L)	--	--	ND
H (atm·m^3/mol)	*H* value was calculated by using the theoretical equation from Lyman, Reehl, and Rosenblatt (1982), which defines the constant. Recommended value was calculated by using the *MW*, *S*, and *Vp* values that are provided in this table.	B-1-6; B-2-6; B-2-8; B-3-6; B-4-6; B-4-12; B-4-19	ND
D_a (cm^2/s)	D_a value was obtained from CHEMDAT8 database (U.S. EPA 1994d).	B-1-6; B-2-6; B-3-6; B-4-6; B-4-21	2.62E-02
D_w (cm^2/s)	D_w value was obtained from CHEMDAT8 database (U.S. EPA 1994d).	B-4-20	5.85E-06
K_{ow} (unitless)	Recommended K_{ow} value cited in Karickhoff and Long (1995).	--	3.98E+01
K_{oc} (mL/g)	K_{oc} value was calculated by using the correlation equation with K_{ow} for phthalates and PAHs, / all nonionizing organics except phthalates, PAHs, dioxins, and furans, cited in U.S. EPA (1994c). K_{oc} value was calculated by using the recommended K_{ow} value that is provided in this table.	--	2.51E+01
Kd_s (cm^3/g)	Kd_s value was calculated by using the correlation equation with K_{oc} that is cited in U.S. EPA (1993d) for an assumed organic carbon fraction of 0.01 in soil. Measured organic carbon in soil, specific to site conditions, should be used to calculate Kd_s, because the value varies, depending on the fraction of organic carbon in soil. Recommended Kd_s value was calculated by using the K_{oc} value that is provided in this table.	B-1-3; B-1-4; B-1-5; B-1-6; B-2-3; B-2-4; B-2-5; B-2-6; B-2-10; B-3-3; B-3-4; B-3-5; B-3-6; B-4-3; B-4-4; B-4-5; B-4-6; B-4-10; B-4-11	2.51E-01
Kd_{sw} (L/Kg)	Kd_{sw} value was calculated by using the correlation equation with K_{oc} that is cited in U.S. EPA (1993d) for an assumed organic carbon fraction of 0.075 in suspended sediment. Measured organic carbon in suspended sediment, specific to site conditions, should be used to calculate Kd_{sw}, because the value varies, depending on the fraction of organic carbon in suspended sediment. Recommended Kd_{sw} value was calculated by using the K_{oc} value that is provided in this table.	B-4-16; B-4-18; B-4-24	1.88E+00
Chemical/Physical Properties (Continued)			

TABLE A-3-198

CHEMICAL-SPECIFIC INPUTS FOR 2,4,6 -TRINITROTOLUENE (118-96-7)

Parameter	Reference and Explanation	Equations	Value
Kd_{bs} (cm^3/g)	Kd_{bs} value was calculated by using the correlation equation with K_{oc} that is cited in U.S. EPA (1993d) for an assumed organic carbon fraction of 0.04 in bottom sediment. Measured organic carbon in bottom sediment, specific to site conditions, should be used to calculate Kd_{bs}, because the value varies, depending on the fraction of organic carbon in bottom sediment. Recommended Kd_{bs} value was calculated by using the K_{oc} value that is provided in this table.	B-4-16; B-4-25	1.00E+00
ksg $(year)^{-1}$	*Ksg* value was calculated by using the chemical half-life in soil, as cited in Howard, Boethling, Jarvis, Meylan, and Michalenko (1991)	B-1-1; B-1-2; B-2-1; B-2-2; B-3-1; B-3-2; B-4-1; B-4-2	1.41E+00
Fv (unitless)	*Fv* value was assumed to be 1.0 due to a lack of data.	B-1-1; B-2-1; B-2-7; B-2-8; B-3-1; B-3-7; B-3-8; B-4-1; B-4-8; B-4-9; B-4-12; B-5-1	1.0
Biotransfer Factors for Plants			
RCF $(\frac{\mu g/g\ DW\ plant}{\mu g/mL\ soil\ water})$	*RCF* value was calculated by using the correlation equation with K_{ow} that is cited in Briggs (1982). Recommended value was calculated by using the K_{ow} value that is provided in this table. The value was then converted to a dry weight basis by using a moisture content of 87 percent.	B-2-10	1.03E+01
$Br_{rootveg}$ $(\frac{\mu g/g\ DW\ plant}{\mu g/g\ soil})$	$Br_{rootveg}$ value was calculated by dividing the *RCF* value with the Kd_s value provided in this table.	B-2-10	4.10E+01
Br_{ag} $(\frac{\mu g/g\ DW\ plant}{\mu g/g\ soil})$	Br_{ag} value was calculated by using the correlation equation with K_{ow} that is cited in Travis and Arms (1988). No distinction was made between values for aboveground produce and forage. Recommended value was calculated by using the K_{ow} value that is provided in this table.	B-2-9	4.60E+00
Br_{forage} $(\frac{\mu g/g\ DW\ plant}{\mu g/g\ soil})$	Br_{forage} value was calculated by using the correlation equation with K_{ow} that is cited in Travis and Arms (1988). No distinction was made between values for aboveground produce and forage. Recommended value was calculated by using the K_{ow} value that is provided in this table.	B-3-9	4.60E+00
Bv_{ag} $(\frac{\mu g/g\ DW\ plant}{\mu g/g\ air})$	--	B-2-8	ND
Bv_{forage} $(\frac{\mu g/g\ DW\ plant}{\mu g/g\ air})$	--	B-3-8	ND

TABLE A-3-198

CHEMICAL-SPECIFIC INPUTS FOR 2,4,6 -TRINITROTOLUENE (118-96-7)

Parameter	Reference and Explanation	Equations	Value
Biotransfer Factors for Animals			
Ba_{milk} (day/kg FW)	Ba_{milk} value was calculated by using the correlation equation with K_{ow} that is cited in Travis and Arms (1988). Recommended value was calculated by using the K_{ow} value that is provided in this table.	B-3-11	3.16E-07
Ba_{beef} (day/kg FW)	Ba_{beef} value was calculated by using the correlation equation with K_{ow} that is cited in Travis and Arms (1988). Recommended value was calculated by using the K_{ow} value that is provided in this table.	B-3-10	1.00E-06
Ba_{pork} (day/kg FW)	Ba_{pork} value was calculated by using the fat content ratio of pork to beef (23/19) and multiplying it with the Ba_{beef} value.	B-3-12	1.21E-06
Ba_{egg} (day/kg FW)	Ba_{egg} value was calculated by using the correlation equation with K_{ow} that is cited in California EPA (1993). Recommended value was calculated by using the K_{ow} value that is provided in this table.	B-3-13	3.16E-04
$Ba_{chicken}$ (day/kg FW)	$Ba_{chicken}$ value was calculated by using the fat content ratio of chicken to beef (15/19) and multiplying it with the Ba_{beef} value.	B-3-14	7.89E-07
BCF_{fish} (L/kg FW tissue)	*BCFs* were used for compounds with a log K_{ow} value below 4.0, as cited in U.S. EPA (1995b). BCF_{fish} value calculated using the correlation equation with K_{ow} obtained from Veith, Macek, Petrocelli, and Caroll (1980)—See Appendix A-3.	B-4-26	9.68E+00
BAF_{fish} (L/kg FW)	--	B-4-27	NA
$BSAF_{fish}$ (unitless)	--	B-4-28	NA
Health Benchmarks			
RfD (mg/kg/day)	U.S. EPA (1997b)	C-1-8	5.0E-04
Oral CSF $(mg/kg/day)^{-1}$	U.S. EPA (1997b)	C-1-7	3.0E-02
RfC (mg/m^3)	Calculated from *RfD* using an inhalation rate of 20 m^3/day and a human body weight of 70 kg.	C-2-3	1.8E-03
Inhalation URF $(\mu g/m^3)^{-1}$	Calculated from *Oral CSF* using an inhalation rate of 20 m^3/day and a human body weight of 70 kg.	C-2-1	8.6E-06
Inhalation CSF $(mg/kg/day)^{-1}$	U.S. EPA (1997b)	C-2-2	3.0E-02

Note:

NA = Not applicable
ND = No data available

All parameters are defined in list of FATE AND TRANSPORT PARAMETERS on page A-3-iii.

TABLE A-3-199

CHEMICAL-SPECIFIC INPUTS FOR VINYL ACETATE (108-05-4)

Parameter	Reference and Explanation	Equations	Value
Chemical/Physical Properties			
MW (g/mole)	Budavari, O'Neil, Smith, and Heckelman (1989)	--	86.09
T_m (K)	Budavari, O'Neil, Smith, and Heckelman (1989)	--	180.1
Vp (atm)	Geometric mean value cited in U.S. EPA (1994c).	--	1.43E-01 at 25°C (liquid)
S (mg/L)	Geometric mean value cited in U.S. EPA (1994c).	--	2.24E+04
H (atm·m^3/mol)	*H* value was calculated by using the theoretical equation from Lyman, Reehl, and Rosenblatt (1982), which defines the constant. Recommended value was calculated by using the *MW*, *S*, and *Vp* values that are provided in this table.	B-1-6; B-2-6; B-2-8; B-3-6; B-4-6; B-4-12; B-4-19	5.50E-04
D_a (cm^2/s)	D_a value was obtained from CHEMDAT8 database (U.S. EPA 1994d).	B-1-6; B-2-6; B-3-6; B-4-6; B-4-21	9.94E-02
D_w (cm^2/s)	D_w value was obtained from CHEMDAT8 database (U.S. EPA 1994d).	B-4-20	1.00E-05
K_{ow} (unitless)	Geometric mean value cited in U.S. EPA (1994c).	--	5.00E+00
K_{oc} (mL/g)	K_{oc} value was calculated by using the correlation equation with K_{ow} for all nonionizing organics except phthalates, PAHs, dioxins, and furans, cited in U.S. EPA (1994c). K_{oc} value was calculated by using the recommended K_{ow} value that is provided in this table.	--	4.97E+00
Kd_s (cm^3/g)	Kd_s value was calculated by using the correlation equation with K_{oc} that is cited in U.S. EPA (1993d) for an assumed organic carbon fraction of 0.01 in soil. Measured organic carbon in soil, specific to site conditions, should be used to calculate Kd_s, because the value varies, depending on the fraction of organic carbon in soil. Recommended Kd_s value was calculated by using the K_{oc} value that is provided in this table.	B-1-3; B-1-4; B-1-5; B-1-6; B-2-3; B-2-4; B-2-5; B-2-6; B-2-10; B-3-3; B-3-4; B-3-5; B-3-6; B-4-3; B-4-4; B-4-5; B-4-6; B-4-10; B-4-11	4.97E-02
Kd_{sw} (L/Kg)	Kd_{sw} value was calculated by using the correlation equation with K_{oc} that is cited in U.S. EPA (1993d) for an assumed organic carbon fraction of 0.075 in suspended sediment. Measured organic carbon in suspended sediment, specific to site conditions, should be used to calculate Kd_{sw}, because the value varies, depending on the fraction of organic carbon in suspended sediment. Recommended Kd_{sw} value was calculated by using the K_{oc} value that is provided in this table.	B-4-16; B-4-18; B-4-24	3.73E-01
Kd_{bs} (cm^3/g)	Kd_{bs} value was calculated by using the correlation equation with K_{oc} that is cited in U.S. EPA (1993d) for an assumed organic carbon fraction of 0.04 in bottom sediment. Measured organic carbon in bottom sediment, specific to site conditions, should be used to calculate Kd_{bs}, because the value varies, depending on the fraction of organic carbon in bottom sediment. Recommended Kd_{bs} value was calculated by using the K_{oc} value that is provided in this table.	B-4-16; B-4-25	1.99E-01
Chemical/Physical Properties (Continued)			
ksg (year)$^{-1}$	*Ksg* value was assumed to be 0 due to a lack of data.	B-1-2; B-2-2; B-3-2; B-4-2	0.0
Fv (unitless)	*Fv* value was calculated by using the equation cited in Junge (1977). Recommended	B-1-1; B-2-1;	1.0

TABLE A-3-199

CHEMICAL-SPECIFIC INPUTS FOR VINYL ACETATE (108-05-4)

Parameter	Reference and Explanation	Equations	Value
Biotransfer Factors for Plants			
RCF ($\frac{\mu g/g\ DW\ plant}{\mu g/mL\ soil\ water}$)	*RCF* value was calculated by using the correlation equation with K_{ow} that is cited in Briggs (1982). Recommended value was calculated by using the K_{ow} value that is provided in this table. The value was then converted to a dry weight basis by using a moisture content of 87 percent.	B-2-10	7.11E+00
$Br_{root\ veg}$ ($\frac{\mu g/g\ DW\ plant}{\mu g/g\ soil}$)	$Br_{root\ veg}$ value was calculated by dividing the *RCF* value with the Kd_s value provided in this table.	B-2-10	1.43E+02
Br_{ag} ($\frac{\mu g/g\ DW\ plant}{\mu g/g\ soil}$)	Br_{ag} value was calculated by using the correlation equation with K_{ow} that is cited in Travis and Arms (1988). No distinction was made between values for aboveground produce and forage. Recommended value was calculated by using the K_{ow} value that is provided in this table.	B-2-9	1.53E+01
Br_{forage} ($\frac{\mu g/g\ DW\ plant}{\mu g/g\ soil}$)	Br_{forage} value was calculated by using the correlation equation with K_{ow} that is cited in Travis and Arms (1988). No distinction was made between values for abovegroud produce and forage. Recommended value was calculated by using the K_{ow} value that is provided in this table.	B-3-9	1.53E+01
Bv_{ag} ($\frac{\mu g/g\ DW\ plant}{\mu g/g\ air}$)	Bv_{ag} value was calculated by using the correlation equation with K_{ow} and *H* that is cited in Bacci, Calamari, Gaggi, and Vighi (1990); and Bacci, Cerejeira, Gaggi, Chemello, Calamari, and Vighi (1992); then reducing this value by a factor of 100. No distinction was made between values for aboveground produce and forage. Recommended value was calculated, for a temperature (T) of 25°C, by using the *H* and K_{ow} values that are provided in this table.	B-2-8	5.65E-04
Bv_{forage} ($\frac{\mu g/g\ DW\ plant}{\mu g/g\ air}$)	Bv_{forage} value was calculated by using the correlation equation with K_{ow} and *H* that is cited in Bacci, Calamari, Gaggi, and Vighi (1990); and Bacci, Cerejeira, Gaggi, Chemello, Calamari, and Vighi (1992); then reducing this value by a factor of 100. No distinction was made between values for aboveground produce and forage. Recommended value was calculated, for a temperature (T) of 25°C, by using the *H* and K_{ow} values that are provided in this table.	B-3-8	5.65E-04
Biotransfer Factors for Animals			
Ba_{milk} (day/kg FW)	Ba_{milk} value was calculated by using the correlation equation with K_{ow} that is cited in Travis and Arms (1988). Recommended value was calculated by using the K_{ow} value that is provided in this table.	B-3-11	3.97E-08
Ba_{beef} (day/kg FW)	Ba_{beef} value was calculated by using the correlation equation with K_{ow} that is cited in Travis and Arms (1988). Recommended value was calculated by using the K_{ow} value that is provided in this table.	B-3-10	1.26E-07
Ba_{pork} (day/kg FW)	Ba_{pork} value was calculated by using the fat content ratio of pork to beef (23/19) and multiplying it with the Ba_{beef} value.	B-3-12	1.52E-07
Ba_{egg} (day/kg FW)	Ba_{egg} value was calculated by using the correlation equation with K_{ow} that is cited in California EPA (1993). Recommended value was calculated by using the K_{ow} value that is provided in this table.	B-3-13	3.97E-05
$Ba_{chicken}$ (day/kg FW)	$Ba_{chicken}$ value was calculated by using the fat content ratio of chicken to beef (15/19) and multiplying it with the Ba_{beef} value.	B-3-14	9.92E-08

TABLE A-3-199

CHEMICAL-SPECIFIC INPUTS FOR VINYL ACETATE (108-05-4)

Parameter	Reference and Explanation	Equations	Value
BCF_{fish} (L/kg FW tissue)	*BCFs* were used for compounds with a log K_{ow} value below 4.0, as cited in U.S. EPA (1995b). BCF_{fish} value calculated using the correlation equation with K_{ow} obtained from Veith, Macek, Petrocelli, and Caroll (1980)—See Appendix A-3.	B-4-26	2.00E+00
BAF_{fish} (L/kg FW)	--	B-4-27	NA
$BSAF_{fish}$ (unitless)	--	B-4-28	NA
Health Benchmarks			
RfD (mg/kg/day)	U.S. EPA (1997c)	C-1-8	1.0E+00
Oral CSF $(mg/kg/day)^{-1}$	--	C-1-7	ND
RfC (mg/m^3)	U.S. EPA (1997b)	C-2-3	2.0E-01
Inhalation URF $(\mu g/m^3)^{-1}$	--	C-2-1	ND
Inhalation CSF $(mg/kg/day)^{-1}$	--	C-2-2	ND

Note:

NA= Not applicable
ND= No data available

All parameters are defined in list of FATE AND TRANSPORT PARAMETERS on page A-3-iii.

TABLE A-3-200

CHEMICAL-SPECIFIC INPUTS FOR VINYL CHLORIDE (75-01-4)

Parameter	Reference and Explanation	Equations	Value
Chemical/Physical Properties			
MW (g/mole)	Budavari, O'Neil, Smith, and Heckelman (1989)	--	62.50
T_m (K)	Budavari, O'Neil, Smith, and Heckelman (1989)	--	119.3
Vp (atm)	Geometric mean value cited in U.S. EPA (1994c).	--	3.68E+00 at 25°C (liquid)
S (mg/L)	Geometric mean value cited in U.S. EPA (1994c).	--	7.30E+02
H (atm·m^3/mol)	*H* value was calculated by using the theoretical equation from Lyman, Reehl, and Rosenblatt (1982), which defines the constant. Recommended value was calculated by using the *MW*, *S*, and *Vp* values that are provided in this table.	B-1-6; B-2-6; B-2-8; B-3-6; B-4-6; B-4-12; B-4-19	3.15E-01
D_a (cm^2/s)	D_a value was obtained from CHEMDAT8 database (U.S. EPA 1994d).	B-1-6; B-2-6; B-3-6; B-4-6; B-4-21	1.58E-01
D_w (cm^2/s)	D_w value was obtained from CHEMDAT8 database (U.S. EPA 1994d).	B-4-20	1.19E-05
K_{ow} (unitless)	Geometric mean value cited in U.S. EPA (1994c).	--	1.40E+01
K_{oc} (mL/g)	K_{oc} value was calculated by using the correlation equation with K_{ow} for all nonionizing organics except phthalates, PAHs, dioxins, and furans as cited in U.S. EPA (1994c). K_{oc} value was calculated by using the recommended K_{ow} value that is provided in this table.	--	1.11E+02
Kd_s (cm^3/g)	Kd_s value was calculated by using the correlation equation with K_{oc} that is cited in U.S. EPA (1993d) for an assumed fraction organic carbon of 0.01 in soil. Measured organic carbon in soil, specific to site conditions, should be used to calculate Kd_s, because the value varies, depending on the fraction of organic carbon in soil. Recommended Kd_s value was calculated by using the K_{oc} value that is provided in this table.	B-1-3; B-1-4; B-1-5; B-1-6; B-2-3; B-2-4; B-2-5; B-2-6; B-2-10; B-3-3; B-3-4; B-3-5; B-3-6; B-4-3; B-4-4; B-4-5; B-4-6; B-4-10; B-4-11	1.11E-01
Kd_{sw} (L/Kg)	Kd_{sw} value was calculated by using the correlation equation with K_{oc} that is cited in U.S. EPA (1993d) for an assumed organic carbon fraction of 0.075 in suspended sediment. Measured organic carbon in suspended sediment, specific to site conditions, should be used to calculate Kd_{sw}, because the value varies, depending on the fraction of organic carbon in suspended sediment. Recommended Kd_{sw} value was calculated by using the K_{oc} value that is provided in this table.	B-4-16; B-4-18; B-4-24	8.32E-01
Kd_{bs} (cm^3/g)	Kd_{bs} value was calculated by using the correlation equation with K_{oc} that is cited in U.S. EPA (1993d) for an assumed organic carbon of 0.04 in bottom sediment. Measured organic carbon in bottom sediment, specific to site conditions, should be used to calculate Kd_{bs}, because the value varies depending on the fraction of organic fraction in bottom sediment. Recommended Kd_{bs} value was calculated by using the K_{oc} value that is provided in this table.	B-4-16; B-4-25	4.44E-01
ksg (year)$^{-1}$	*Ksg* value was calculated by using the chemical half-life in soil, as cited in Howard, Boethling, Jarvis, Meylan, and Michalenko (1991).	B-1-2; B-2-2; B-3-2; B-4-2	1.41E+00

TABLE A-3-200

CHEMICAL-SPECIFIC INPUTS FOR VINYL CHLORIDE (75-01-4)

Parameter	Reference and Explanation	Equations	Value
Fv (unitless)	*Fv* value was calculated by using the equation cited in Junge (1977). Recommended value of *Fv* was calculated by using the *Vp* value that is provided in this table.	B-1-1; B-2-1; B-2-7; B-2-8; B-3-1; B-3-7; B-3-8; B-4-1; B-4-8; B-4-9; B-4-12; B-5-1	1.0
Biotransfer Factors for Plants			
RCF $(\frac{\mu g/g\ DW\ plant}{\mu g/mL\ soil\ water})$	*RCF* value was calculated by using the correlation equation with K_{ow} that is cited in Briggs (1982). Recommended value was calculated by using the K_{ow} value that is provided in this table. The value was converted to a dry weight basis by using a moisture content of 87 percent.	B-2-10	8.08E+00
$Br_{root\ veg}$ $(\frac{\mu g/g\ DW\ plant}{\mu g/g\ soil})$	$Br_{root\ veg}$ value was calculated by dividing the *RCF* value with the Kd_s value provided in this table (see section A4.3.2 of Appendix A-3).	B-2-10	7.29E+01
Br_{ag} $(\frac{\mu g/g\ DW\ plant}{\mu g/g\ soil})$	Br_{ag} value was calculated by using the correlation equation with K_{ow} that is cited in Travis and Arms (1988). No distinction was made between values for aboveground produce and forage. Recommended value was calculated by using the K_{ow} value that is provided in this table.	B-2-9	8.42E+00
Br_{forage} $(\frac{\mu g/g\ DW\ plant}{\mu g/g\ soil})$	Br_{forage} value was calculated by using the correlation equation with K_{ow} that is cited in Travis and Arms (1988). No distinction was made between values for aboveground produce and forage. Recommended value was calculated by using the K_{ow} value that is provided in this table.	B-3-9	8.42E+00
Bv_{ag} $(\frac{\mu g/g\ DW\ plant}{\mu g/g\ air})$	Bv_{ag} value was calculated by using the correlation equation with K_{ow} and *H* that is cited in Bacci and others (1990; 1992); then reducing this value by a factor of 100, as recommended by U.S. EPA (1993d). No distinction was made between values for aboveground produce and forage. Recommended value was calculated, for a temperature (T) of 25°C, by using the *H* and K_{ow} values that are provided in this table.	B-2-8	2.95E-06
Bv_{forage} $(\frac{\mu g/g\ DW\ plant}{\mu g/g\ air})$	Bv_{forage} value was calculated by using the correlation equation with K_{ow} and *H* that is cited in Bacci, Calamari, Gaggi, and Vighi (1990); and Bacci, Cerejeira, Gaggi, Chemello, Calamari, and Vighi (1992); then reducing this value by a factor of 100, as recommended by U.S. EPA (1993d). No distinction was made between values for aboveground produce and forage. Recommended value was calculated, for a temperature (T) of 25°C, by using the *H* and K_{ow} values that are provided in this table.	B-3-8	2.95E-06
Biotransfer Factors for Animals			
Ba_{milk} (day/kg FW)	Ba_{milk} value was calculated by using the correlation equation with K_{ow} that is cited in Travis and Arms (1988). Recommended value was calculated by using the K_{ow} value that is provided in this table.	B-3-11	1.11E-07
Ba_{beef} (day/kg FW)	Ba_{beef} value was calculated by using the correlation equation with K_{ow} that is cited in Travis and Arms (1988). Recommended value was calculated by using the K_{ow} value that is provided in this table.	B-3-10	3.52E-07
Ba_{pork} (day/kg FW)	Ba_{pork} value was calculated by using thethe fat content ratio of pork to beef (23/19) and multiplying it with the Ba_{beef} value (see section A4.3.2 of Appendix A-3).	B-3-12	4.26E-07

TABLE A-3-200

CHEMICAL-SPECIFIC INPUTS FOR VINYL CHLORIDE (75-01-4)

Parameter	Reference and Explanation	Equations	Value
Ba_{eggs} (day/kg FW)	Ba_{eggs} value was calculated by using the correlation equation with K_{ow} that is cited in California EPA (1993). Recommended value was calculated by using the K_{ow} value that is provided in this table.	B-3-13	1.11E-04
$Ba_{chicken}$ (day/kg FW)	$Ba_{chicken}$ value was calculated by using the fat content ratio of chicken to beef (15/19) and multiplying it with the Ba_{beef} value (see section A4.3.2 of Appendix A-3).	B-3-14	2.78E-07
BCF_{fish} (L/kg, FW tissue)	*BAFs* were used for compounds with a log K_{ow} value above 4.0, as cited in U.S. EPA (1995b). *BAF* values were predicted values calculated by multiplying a food chain multiplier (*FCM*) with a geometric mean of various laboratory measured *BCF*s obtained from various experimental studies cited in U.S. EPA (1998). *FCM*s were obtained from U.S. EPA (1995bc)—See Appendix A-3.	B-4-26	4.37E+00
BAF_{fish} (L/kg FW)	--	B-4-27	NA
$BSAF_{fish}$ (unitless)	--	B-4-28	NA
Health Benchmarks			
RfD (mg/kg/day)	--	C-1-8	ND
Oral CSF $(mg/kg/day)^{-1}$	U.S. EPA (1997c)	C-1-7	1.9E+00
RfC (mg/m^3)	--	C-2-3	ND
Inhalation URF $(\mu g/m^3)^{-1}$	U.S. EPA (1997c)	C-2-1	8.4E-05
Inhalation CSF $(mg/kg/day)^{-1}$	U.S. EPA (1997c)	C-2-2	3.0E-01

Note:

NA = Not applicable
ND = No data available

All parameters are defined in list of FATE AND TRANSPORT PARAMETERS on page A-3-iii.

TABLE A-3-201

CHEMICAL-SPECIFIC INPUTS FOR *M*-XYLENE (1330-20-7)

Parameter	Reference and Explanation	Equations	Value
Chemical/Physical Properties			
MW (g/mole)	Budavari, O'Neil, Smith, and Heckelman (1989)	--	106.16
T_m (K)	Montgomery and Welkom (1991)	--	225.7
Vp (atm)	*Vp* value cited in U.S. EPA (1992a).	--	1.39E-05 at 25°C (liquid)
S (mg/L)	*S* value cited in U.S. EPA (1992a).	--	1.60E+02
H (atm·m^3/mol)	*H* value was calculated by using the theoretical equation from Lyman, Reehl, and Rosenblatt (1982), which defines the constant. Recommended value was calculated by using the *MW*, *S*, and *Vp* values that are provided in this table.	B-1-6; B-2-6; B-2-8; B-3-6; B-4-6; B-4-12; B-4-19	9.26E-06
D_a (cm^2/s)	D_a value was obtained from CHEMDAT8 database (U.S. EPA 1994d).	B-1-6; B-2-6; B-3-6; B-4-6; B-4-21	7.69E-02
D_w (cm^2/s)	D_w value was obtained from CHEMDAT8 database (U.S. EPA 1994d).	B-4-20	8.49E-06
K_{ow} (unitless)	Recommended K_{ow} value cited in Karickhoff and Long (1995).	--	1.59E+03
K_{oc} (mL/g)	Geometric mean of measured values obtained from U.S. EPA (1996b).	--	1.96E+02
Kd_s (cm^3/g)	Kd_s value was calculated by using the correlation equation with K_{oc} that is cited in U.S. EPA (1993d) for an assumed organic carbon fraction of 0.01 in soil. Measured organic carbon in soil, specific to site conditions, should be used to calculate Kd_s, because the value varies, depending on the fraction of organic carbon in soil. Recommended Kd_s value was calculated by using the K_{oc} value that is provided in this table.	B-1-3; B-1-4; B-1-5; B-1-6; B-2-3; B-2-4; B-2-5; B-2-6; B-2-10; B-3-3; B-3-4; B-3-5; B-3-6; B-4-3; B-4-4; B-4-5; B-4-6; B-4-10; B-4-11	1.96E+00
Kd_{sw} (L/Kg)	Kd_{sw} value was calculated by using the correlation equation with K_{oc} that is cited in U.S. EPA (1993d) for an assumed organic carbon fraction of 0.075 in suspended sediment. Measured organic carbon in suspended sediment, specific to site conditions, should be used to calculate Kd_{sw}, because the value varies, depending on the fraction of organic carbon in suspended sediment. Recommended Kd_{sw} value was calculated by using the K_{oc} value that is provided in this table.	B-4-16; B-4-18; B-4-24	1.47E+01
Kd_{bs} (cm^3/g)	Kd_{bs} value was calculated by using the correlation equation with K_{oc} that is cited in U.S. EPA (1993d) for an assumed organic carbon fraction of 0.04 in bottom sediment. Measured organic carbon in bottom sediment, specific to site conditions, should be used to calculate Kd_{bs}, because the value varies, depending on the fraction of organic carbon in bottom sediment. Recommended Kd_{bs} value was calculated by using the K_{oc} value that is provided in this table.	B-4-16; B-4-25	7.84E+00
Chemical/Physical Properties (Continued)			
ksg (year)$^{-1}$	*Ksg* value was calculated by using the chemical half-life in soil, as cited in Howard, Boethling, Jarvis, Meylan, and Michalenko (1991).	B-1-1; B-1-2; B-2-1; B-2-2; B-3-1; B-3-2; B-4-1; B-4-2	9.03E+00
Fv (unitless)	*Fv* value was calculated by using the equation cited in Junge (1977). Recommended value of *Fv* was calculated by using the *Vp* value that is provided in the table.	B-1-1; B-2-1; B-2-7; B-2-8;	1.000

TABLE A-3-201

CHEMICAL-SPECIFIC INPUTS FOR *M*-XYLENE (1330-20-7)

Parameter	Reference and Explanation	Equations	Value
Biotransfer Factors for Plants			
RCF $(\frac{\mu g/g\ DW\ plant}{\mu g/mL\ soil\ water})$	*RCF* value was calculated by using the correlation equation with K_{ow} that is cited in Briggs (1982). Recommended value was calculated by using the K_{ow} value that is provided in this table. The value was then converted to a dry weight basis by using a moisture content of 87 percent.	--	7.41E+01
$Br_{rootveg}$ $(\frac{\mu g/g\ DW\ plant}{\mu g/g\ soil})$	$Br_{rootveg}$ value was calculated by dividing the *RCF* value with the Kd_s value provided in this table.	B-2-10	3.78E+01
Br_{ag} $(\frac{\mu g/g\ DW\ plant}{\mu g/g\ soil})$	Br_{ag} value was calculated by using the correlation equation with K_{ow} that is cited in Travis and Arms (1988). No distinction was made between values for aboveground produce and forage. Recommended value was calculated by using the K_{ow} value that is provided in this table.	B-2-9	5.47E-01
Br_{forage} $(\frac{\mu g/g\ DW\ plant}{\mu g/g\ soil})$	Br_{forage} value was calculated by using the correlation equation with K_{ow} that is cited in Travis and Arms (1988). No distinction was made between values for abovegroud produce and forage. Recommended value was calculated by using the K_{ow} value that is provided in this table.	B-3-9	5.47E-01
Bv_{ag} $(\frac{\mu g/g\ DW\ plant}{\mu g/g\ air})$	Bv_{ag} value was calculated by using the correlation equation with K_{ow} and *H* that is cited in Bacci, Calamari, Gaggi, and Vighi (1990); and Bacci, Cerejeira, Gaggi, Chemello, Calamari, and Vighi (1992); then reducing this value by a factor of 100. No distinction was made between values for aboveground produce and forage. Recommended value was calculated, for a temperature (T) of 25ºC, by using the *H* and K_{ow} values that are provided in this table.	B-2-8	1.55E+01
Bv_{forage} $(\frac{\mu g/g\ DW\ plant}{\mu g/g\ air})$	Bv_{forage} value was calculated by using the correlation equation with K_{ow} and *H* that is cited in Bacci, Calamari, Gaggi, and Vighi (1990); and Bacci, Cerejeira, Gaggi, Chemello, Calamari, and Vighi (1992); then reducing this value by a factor of 100. No distinction was made between values for aboveground produce and forage. Recommended value was calculated, for a temperature (T) of 25ºC, by using the *H* and K_{ow} values that are provided in this table.	B-3-8	1.55E+01
Biotransfer Factors for Animals			
Ba_{milk} (day/kg FW)	Ba_{milk} value was calculated by using the correlation equation with K_{ow} that is cited in Travis and Arms (1988). Recommended value was calculated by using the K_{ow} value that is provided in this table.	B-3-11	1.26E-05
Ba_{beef} (day/kg FW)	Ba_{beef} value was calculated by using the correlation equation with K_{ow} that is cited in Travis and Arms (1988). Recommended value was calculated by using the K_{ow} value that is provided in this table.	B-3-10	3.99E-05
Ba_{pork} (day/kg FW)	Ba_{pork} value was calculated by using the fat content ratio of pork to beef (23/19) and multiplying it with the Ba_{beef} value.	B-3-12	4.83E-05
Ba_{egg} (day/kg FW)	Ba_{egg} value was calculated by using the correlation equation with K_{ow} that is cited in California EPA (1993). Recommended value was calculated by using the K_{ow} value that is provided in this table.	B-3-13	1.26E-02
$Ba_{chicken}$ (day/kg FW)	$Ba_{chicken}$ value was calculated by using the fat content ratio of chicken to beef (15/19) and multiplying it with the Ba_{beef} value.	B-3-14	3.15E-05

TABLE A-3-201

CHEMICAL-SPECIFIC INPUTS FOR *M*-XYLENE (1330-20-7)

Parameter	Reference and Explanation	Equations	Value
BCF_{fish} (L/kg FW tissue)	*BCFs* were used for compounds with a log K_{ow} value below 4.0, as cited in U.S. EPA (1995b). BCF_{fish} value calculated using the correlation equation with K_{ow} obtained from Veith, Macek, Petrocelli, and Caroll (1980)—See Appendix A-3.	B-4-26	1.60E+02
BAF_{fish} (L/kg FW)	--	B-4-27	NA
$BSAF_{fish}$ (unitless)	--	B-4-28	NA
Health Benchmarks			
RfD (mg/kg/day)	U.S.EPA (1997b)	C-1-8	2.0E+00
Oral CSF $(mg/kg/day)^{-1}$	--	C-1-7	ND
RfC (mg/m^3)	Calculated from *RfD* using an inhalation rate of 20 m^3/day and a human body weight of 70 kg.	C-2-3	7.0E+00
Inhalation URF $(\mu g/m^3)^{-1}$	--	C-2-1	ND
Inhalation CSF $(mg/kg/day)^{-1}$	--	C-2-2	ND

Note:

NA = Not applicable
ND = No data available

All parameters are defined in list of FATE AND TRANSPORT PARAMETERS on page A-3-iii.

TABLE A-3-202

CHEMICAL-SPECIFIC INPUTS FOR *O*-XYLENE (1330-20-7)

Parameter	Reference and Explanation	Equations	Value
Chemical/Physical Properties			
MW (g/mole)	Budavari, O'Neil, Smith, and Heckelman (1989)	--	106.16
T_m (K)	Montgomery and Welkom (1991)	--	248.1
Vp (atm)	*Vp* value cited in U.S. EPA (1992a).	--	1.39E-05 at 25°C (liquid)
S (mg/L)	*S* value cited in U.S. EPA (1992a).	--	2.20E+02
H (atm·m^3/mol)	*H* value was calculated by using the theoretical equation from Lyman, Reehl, and Rosenblatt (1982), which defines the constant. Recommended value was calculated by using the *MW*, *S*, and *Vp* values that are provided in this table.	B-1-6; B-2-6; B-2-8; B-3-6; B-4-6; B-4-12; B-4-19	6.73E-06
D_a (cm^2/s)	D_a value was obtained from CHEMDAT8 database (U.S. EPA 1994d).	B-1-6; B-2-6; B-3-6; B-4-6; B-4-21	7.69E-02
D_w (cm^2/s)	D_w value was obtained from CHEMDAT8 database (U.S. EPA 1994d).	B-4-20	8.44E-06
K_{ow} (unitless)	Recommended K_{ow} value cited in Karickhoff and Long (1995).	--	1.35E+03
K_{oc} (mL/g)	Geometric mean of measured values obtained from U.S. EPA (1996b).	--	2.41E+02
Kd_s (cm^3/g)	Kd_s value was calculated by using the correlation equation with K_{oc} that is cited in U.S. EPA (1993d) for an assumed organic carbon fraction of 0.01 in soil. Measured organic carbon in soil, specific to site conditions, should be used to calculate Kd_s, because the value varies, depending on the fraction of organic carbon in soil. Recommended Kd_s value was calculated by using the K_{oc} value that is provided in this table.	B-1-3; B-1-4; B-1-5; B-1-6; B-2-3; B-2-4; B-2-5; B-2-6; B-2-10; B-3-3; B-3-4; B-3-5; B-3-6; B-4-3; B-4-4; B-4-5; B-4-6; B-4-10; B-4-11	2.41E+00
Kd_{sw} (L/Kg)	Kd_{sw} value was calculated by using the correlation equation with K_{oc} that is cited in U.S. EPA (1993d) for an assumed organic carbon fraction of 0.075 in suspended sediment. Measured organic carbon in suspended sediment, specific to site conditions, should be used to calculate Kd_{sw}, because the value varies, depending on the fraction of organic carbon in suspended sediment. Recommended Kd_{sw} value was calculated by using the K_{oc} value that is provided in this table.	B-4-16; B-4-18; B-4-24	1.81E+01
Kd_{bs} (cm^3/g)	Kd_{bs} value was calculated by using the correlation equation with K_{oc} that is cited in U.S. EPA (1993d) for an assumed organic carbon fraction of 0.04 in bottom sediment. Measured organic carbon in bottom sediment, specific to site conditions, should be used to calculate Kd_{bs}, because the value varies, depending on the fraction of organic carbon in bottom sediment. Recommended Kd_{bs} value was calculated by using the K_{oc} value that is provided in this table.	B-4-16; B-4-25	9.64E+00
Chemical/Physical Properties (Continued)			
ksg (year)$^{-1}$	*Ksg* value was calculated by using the chemical half-life in soil, as cited in Howard, Boethling, Jarvis, Meylan, and Michalenko (1991).	B-1-1; B-1-2; B-2-1; B-2-2; B-3-1; B-3-2; B-4-1; B-4-2	9.03E+00
Fv (unitless)	*Fv* value was calculated by using the equation cited in Junge (1977). Recommended value of *Fv* was calculated by using the *Vp* value that is provided in the table.	B-1-1; B-2-1; B-2-7; B-2-8;	1.000

TABLE A-3-202

CHEMICAL-SPECIFIC INPUTS FOR *O*-XYLENE (1330-20-7)

Parameter	Reference and Explanation	Equations	Value
Biotransfer Factors for Plants			
RCF $(\frac{\mu g/g\ DW\ plant}{\mu g/mL\ soil\ water})$	*RCF* value was calculated by using the correlation equation with K_{ow} that is cited in Briggs (1982). Recommended value was calculated by using the K_{ow} value that is provided in this table. The value was then converted to a dry weight basis by using a moisture content of 87 percent.	--	6.61E+01
$Br_{rootveg}$ $(\frac{\mu g/g\ DW\ plant}{\mu g/g\ soil})$	$Br_{rootveg}$ value was calculated by dividing the *RCF* value with the Kd_s value provided in this table.	B-2-10	2.74E+01
Br_{ag} $(\frac{\mu g/g\ DW\ plant}{\mu g/g\ soil})$	Br_{ag} value was calculated by using the correlation equation with K_{ow} that is cited in Travis and Arms (1988). No distinction was made between values for aboveground produce and forage. Recommended value was calculated by using the K_{ow} value that is provided in this table.	B-2-9	6.01E-01
Br_{forage} $(\frac{\mu g/g\ DW\ plant}{\mu g/g\ soil})$	Br_{forage} value was calculated by using the correlation equation with K_{ow} that is cited in Travis and Arms (1988). No distinction was made between values for abovegroud produce and forage. Recommended value was calculated by using the K_{ow} value that is provided in this table.	B-3-9	6.01E-01
Bv_{ag} $(\frac{\mu g/g\ DW\ plant}{\mu g/g\ air})$	Bv_{ag} value was calculated by using the correlation equation with K_{ow} and *H* that is cited in Bacci, Calamari, Gaggi, and Vighi (1990); and Bacci, Cerejeira, Gaggi, Chemello, Calamari, and Vighi (1992); then reducing this value by a factor of 100. No distinction was made between values for aboveground produce and forage. Recommended value was calculated, for a temperature (T) of 25ºC, by using the *H* and K_{ow} values that are provided in this table.	B-2-8	1.79E+01
Bv_{forage} $(\frac{\mu g/g\ DW\ plant}{\mu g/g\ air})$	Bv_{forage} value was calculated by using the correlation equation with K_{ow} and *H* that is cited in Bacci, Calamari, Gaggi, and Vighi (1990); and Bacci, Cerejeira, Gaggi, Chemello, Calamari, and Vighi (1992); then reducing this value by a factor of 100. No distinction was made between values for aboveground produce and forage. Recommended value was calculated, for a temperature (T) of 25ºC, by using the *H* and K_{ow} values that are provided in this table.	B-3-8	1.79E+01
Biotransfer Factors for Animals			
Ba_{milk} (day/kg FW)	Ba_{milk} value was calculated by using the correlation equation with K_{ow} that is cited in Travis and Arms (1988). Recommended value was calculated by using the K_{ow} value that is provided in this table.	B-3-11	1.07E-05
Ba_{beef} (day/kg FW)	Ba_{beef} value was calculated by using the correlation equation with K_{ow} that is cited in Travis and Arms (1988). Recommended value was calculated by using the K_{ow} value that is provided in this table.	B-3-10	3.39E-05
Ba_{pork} (day/kg FW)	Ba_{pork} value was calculated by using the fat content ratio of pork to beef (23/19) and multiplying it with the Ba_{beef} value.	B-3-12	4.10E-05
Ba_{egg} (day/kg FW)	Ba_{egg} value was calculated by using the correlation equation with K_{ow} that is cited in California EPA (1993). Recommended value was calculated by using the K_{ow} value that is provided in this table.	B-3-13	1.07E-02
$Ba_{chicken}$ (day/kg FW)	$Ba_{chicken}$ value was calculated by using the fat content ratio of chicken to beef (15/19) and multiplying it with the Ba_{beef} value.	B-3-14	2.68E-05

TABLE A-3-202

CHEMICAL-SPECIFIC INPUTS FOR *O*-XYLENE (1330-20-7)

Parameter	Reference and Explanation	Equations	Value
BCF_{fish} (L/kg FW tissue)	*BCFs* were used for compounds with a log K_{ow} value below 4.0, as cited in U.S. EPA (1995b). BCF_{fish} value calculated using the correlation equation with K_{ow} obtained from Veith, Macek, Petrocelli, and Caroll (1980)—See Appendix A-3.	B-4-26	1.41E+02
BAF_{fish} (L/kg FW)	--	B-4-27	NA
$BSAF_{fish}$ (unitless)	--	B-4-28	NA
Health Benchmarks			
RfD (mg/kg/day)	U.S.EPA (1997b)	C-1-8	2.0E+00
Oral CSF $(mg/kg/day)^{-1}$	--	C-1-7	ND
RfC (mg/m^3)	Calculated from *RfD* using an inhalation rate of 20 m^3/day and a human body weight of 70 kg.	C-2-3	7.0E+00
Inhalation URF $(\mu g/m^3)^{-1}$	--	C-2-1	ND
Inhalation CSF $(mg/kg/day)^{-1}$	--	C-2-2	ND

Note:

NA = Not applicable
ND = No data available

All parameters are defined in list of FATE AND TRANSPORT PARAMETERS on page A-3-iii.

TABLE A-3-203

CHEMICAL-SPECIFIC INPUTS FOR *P*-XYLENE (1330-20-7)

Parameter	Reference and Explanation	Equations	Value
Chemical/Physical Properties			
MW (g/mole)	Budavari, O'Neil, Smith, and Heckelman (1989)	--	106.16
T_m (K)	Montgomery and Welkom (1991)	--	286.1
Vp (atm)	*Vp* value cited in U.S. EPA (1992a).	--	1.39E-05 at 25°C (liquid)
S (mg/L)	*S* value cited in U.S. EPA (1992a).	--	2.15E+02
H (atm·m^3/mol)	*H* value was calculated by using the theoretical equation from Lyman, Reehl, and Rosenblatt (1982), which defines the constant. Recommended value was calculated by using the *MW*, *S*, and *Vp* values that are provided in this table.	B-1-6; B-2-6; B-2-8; B-3-6; B-4-6; B-4-12; B-4-19	6.89E-06
D_a (cm^2/s)	D_a value was obtained from CHEMDAT8 database (U.S. EPA 1994d).	B-1-6; B-2-6; B-3-6; B-4-6; B-4-21	7.61E+02
D_w (cm^2/s)	D_w value was obtained from CHEMDAT8 database (U.S. EPA 1994d).	B-4-20	8.50E-06
K_{ow} (unitless)	Recommended K_{ow} value cited in Karickhoff and Long (1995).	--	1.48E+03
K_{oc} (mL/g)	Geometric mean of measured values obtained from U.S. EPA (1996b).	--	3.11E+02
Kd_s (cm^3/g)	Kd_s value was calculated by using the correlation equation with K_{oc} that is cited in U.S. EPA (1993d) for an assumed organic carbon fraction of 0.01 in soil. Measured organic carbon in soil, specific to site conditions, should be used to calculate Kd_s, because the value varies, depending on the fraction of organic carbon in soil. Recommended Kd_s value was calculated by using the K_{oc} value that is provided in this table.	B-1-3; B-1-4; B-1-5; B-1-6; B-2-3; B-2-4; B-2-5; B-2-6; B-2-10; B-3-3; B-3-4; B-3-5; B-3-6; B-4-3; B-4-4; B-4-5; B-4-6; B-4-10; B-4-11	3.11E+00
Kd_{sw} (L/Kg)	Kd_{sw} value was calculated by using the correlation equation with K_{oc} that is cited in U.S. EPA (1993d) for an assumed organic carbon fraction of 0.075 in suspended sediment. Measured organic carbon in suspended sediment, specific to site conditions, should be used to calculate Kd_{sw}, because the value varies, depending on the fraction of organic carbon in suspended sediment. Recommended Kd_{sw} value was calculated by using the K_{oc} value that is provided in this table.	B-4-16; B-4-18; B-4-24	2.33E+01
Kd_{bs} (cm^3/g)	Kd_{bs} value was calculated by using the correlation equation with K_{oc} that is cited in U.S. EPA (1993d) for an assumed organic carbon fraction of 0.04 in bottom sediment. Measured organic carbon in bottom sediment, specific to site conditions, should be used to calculate Kd_{bs}, because the value varies, depending on the fraction of organic carbon in bottom sediment. Recommended Kd_{bs} value was calculated by using the K_{oc} value that is provided in this table.	B-4-16; B-4-25	1.24E+01
Chemical/Physical Properties (Continued)			
ksg (year)$^{-1}$	*Ksg* value was calculated by using the chemical half-life in soil, as cited in Howard, Boethling, Jarvis, Meylan, and Michalenko (1991).	B-1-1; B-1-2; B-2-1; B-2-2; B-3-1; B-3-2; B-4-1; B-4-2	9.03E+00
Fv (unitless)	*Fv* value was calculated by using equations cited in Junge (1977) and Bidleman (1988). Recommended value of *Fv* was calculated by using T_m and *Vp* values that	B-1-1; B-2-1; B-2-7; B-2-8;	1.00

TABLE A-3-203

CHEMICAL-SPECIFIC INPUTS FOR *P*-XYLENE (1330-20-7)

Parameter	Reference and Explanation	Equations	Value
Biotransfer Factors for Plants			
RCF $(\frac{\mu g/g\ WW\ plant}{\mu g/mL\ soil\ water})$	*RCF* value was calculated by using the correlation equation with K_{ow} that is cited in Briggs (1982). Recommended value was calculated by using the K_{ow} value that is provided in this table.	B-2-10	7.05E+01
$Br_{rootveg}$ $(\frac{\mu g/g\ WW\ plant}{\mu g/g\ soil})$	$Br_{rootveg}$ value was calculated by dividing the *RCF* value with the Kd_s value provided in this table.	B-2-10	2.27E+01
Br_{ag} $(\frac{\mu g/g\ DW\ plant}{\mu g/g\ soil})$	Br_{ag} value was calculated by using the correlation equation with K_{ow} that is cited in Travis and Arms (1988). No distinction was made between values for aboveground produce and forage. Recommended value was calculated by using the K_{ow} value that is provided in this table.	B-2-9	5.70E-01
Br_{forage} $(\frac{\mu g/g\ DW\ plant}{\mu g/g\ soil})$	Br_{forage} value was calculated by using the correlation equation with K_{ow} that is cited in Travis and Arms (1988). No distinction was made between values for aboveground produce and forage. Recommended value was calculated by using the K_{ow} value that is provided in this table.	B-3-9	5.70E-01
Bv_{ag} $(\frac{\mu g/g\ DW\ plant}{\mu g/g\ air})$	Bv_{ag} value was calculated by using the correlation equation with K_{ow} and *H* that is cited in Bacci, Calamari, Gaggi, and Vighi (1990); and Bacci, Cerejeira, Gaggi, Chemello, Calamari, and Vighi (1992); then reducing this value by a factor of 100, as recommended by U.S. EPA (1993d). No distinction was made between values for aboveground produce and forage. Recommended value was calculated, for a temperature (T) of 25ºC, by using the *H* and K_{ow} values that are provided in this table.	B-2-8	1.93E+01
Bv_{forage} $(\frac{\mu g/g\ DW\ plant}{\mu g/g\ air})$	Bv_{forage} value was calculated by using the correlation equation with K_{ow} and *H* that is cited in Bacci, Calamari, Gaggi, and Vighi (1990); and Bacci, Cerejeira, Gaggi, Chemello, Calamari, and Vighi (1992); then reducing this value by a factor of 100, as recommended by U.S. EPA (1993d). No distinction was made between values for aboveground produce and forage. Recommended value was calculated, for a temperature (T) of 25ºC, by using the *H* and K_{ow} values that are provided in this table.	B-3-8	1.93E+01
Biotransfer Factors for Animals			
Ba_{milk} (day/kg FW)	Ba_{milk} value was calculated by using the correlation equation with K_{ow} that is cited in Travis and Arms (1988). Recommended value was calculated by using the K_{ow} value that is provided in this table.	B-3-11	1.18E-05
Ba_{beef} (day/kg FW)	Ba_{beef} value was calculated by using the correlation equation with K_{ow} that is cited in Travis and Arms (1988). Recommended value was calculated by using the K_{ow} value that is provided in this table.	B-3-10	3.72E-05
Ba_{pork} (day/kg FW)	Ba_{pork} value was calculated by using the fat content ratio of pork to beef (23/19) and multiplying it with the Ba_{beef} value.	B-3-12	4.50E-05
Ba_{egg} (day/kg FW)	Ba_{egg} value was calculated by using the correlation equation with K_{ow} that is cited in California EPA (1993). Recommended value was calculated by using the K_{ow} value that is provided in this table.	B-3-13	1.18E-02
$Ba_{chicken}$ (day/kg FW)	$Ba_{chicken}$ value was calculated by using the fat content ratio of chicken to beef (15/19) and multiplying it with the Ba_{beef} value.	B-3-14	2.93E-05

TABLE A-3-203

CHEMICAL-SPECIFIC INPUTS FOR *P*-XYLENE (1330-20-7)

Parameter	Reference and Explanation	Equations	Value
BCF_{fish} (L/kg FW tissue)	*BCFs* were used for compounds with a log K_{ow} value below 4.0, as cited in U.S. EPA (1995b). BCF_{fish} value calculated using the correlation equation with K_{ow} obtained from Veith, Macek, Petrocelli, and Caroll (1980)—See Appendix A-3.	B-4-26	1.51E+02
BAF_{fish} (L/kg FW)	--	B-4-27	NA
$BSAF_{fish}$ (unitless)	--	B-4-28	NA
Health Benchmarks			
RfD (mg/kg/day)	U.S.EPA (1997b)	C-1-8	2.0E+00
Oral CSF $(mg/kg/day)^{-1}$	--	C-1-7	ND
RfC (mg/m^3)	Calculated from *RfD* using an inhalation rate of 20 m^3/day and a human body weight of 70 kg.	C-2-3	7.0E+00
Inhalation URF $(\mu g/m^3)^{-1}$	--	C-2-1	ND
Inhalation CSF $(mg/kg/day)^{-1}$	--	C-2-2	ND

Note:

NA = Not applicable
ND = No data available

All parameters are defined in list of FATE AND TRANSPORT PARAMETERS on page A-3-iii.

TABLE A-3-204

CHEMICAL-SPECIFIC INPUTS FOR ZINC (7440-66-6)

Parameter	Reference and Explanation	Equations	Value
Chemical/Physical Properties			
MW (g/mole)	Budavari, O'Neil, Smith, and Heckelman (1989)	--	65.38
T_m (^{o}K)	Budavari, O'Neil, Smith, and Heckelman (1989)	--	692.6
Vp (atm)	All metals, except mercury, are assumed to be nonvolatile at ambient temperatures.	--	0.0
S (mg/L)	All metals, except mercury, are assumed to be insoluble in water. OR Budavari, O'Neil, Smith, and Heckelman (1989)	--	0.0
H (atm·m^3/mol)	*H* value is assumed to be zero, because the *Vp* and *S* values are zero for all metals, except mercury.	B-1-6; B-2-6; B-2-8; B-3-6; B-4-6; B-4-12; B-4-19	0.0
D_a (cm^2/s)	D_a value was calculated using the equation cited in U.S. EPA (1996a).	B-1-6; B-2-6; B-3-6; B-4-6; B-4-21	1.17E-01
D_w (cm^2/s)	D_w value was calculated using the equation cited in U.S. EPA (1996a).	B-4-20	1.36E-05
K_{ow} (unitless)	--	--	NA
K_{oc} (mL/g)	--	--	NA
Kd_s (mL/g)	Kd_s value was obtained from U.S. EPA (1996), which provides pH-based values that were estimated by using the MINTEQ2 geochemical speciation model.	B-1-3; B-1-4; B-1-5; B-1-6; B-2-3; B-2-4; B-2-5; B-2-6; B-2-10; B-3-3; B-3-4; B-3-5; B-3-6; B-4-3; B-4-4; B-4-5; B-4-6; B-4-10; B-4-11	6.2E+01 at pH=6.8
Kd_{sw} (L/Kg)	Kd_{sw} value is assumed to be same as the Kd_s value, because organic carbon does not play a major role in sorption for the metals, as cited in U.S. EPA (1994f).	B-4-16; B-4-18; B-4-24	6.2E+01 at pH=6.8
Kd_{bs} (mL/g)	Kd_{bs} value is assumed to be same as the Kd_s value, because organic carbon does not play a major role in sorption for the metals, as cited in U.S. EPA (1994f).	B-4-16; B-4-25	6.2E+01 at pH=6.8
ksg (year)$^{-1}$	--	B-1-1; B-1-2; B-2-1; B-2-2; B-3-1; B-3-2; B-4-1; B-4-2	ND

TABLE A-3-204

CHEMICAL-SPECIFIC INPUTS FOR ZINC (7440-66-6)

Parameter	Reference and Explanation	Equations	Value
Chemical/Physical Properties (Continued)			
Fv (unitless)	Because they are nonvolatile, metals are assumed to be 100 percent in particulate phase and zero percent in the vapor phase, as cited in U.S. EPA (1994f).	B-1-1; B-2-1; B-2-7; B-2-8; B-3-1; B-3-7; B-3-8; B-4-1; B-4-8; B-4-9; B-4-12; B-5-1	0.0
Biotransfer Factors for Plants			
RCF $(\frac{\mu g/g\ DW\ plant}{\mu g/mL\ soil\ water})$	--	--	ND
$Br_{rootveg}$ $(\frac{\mu g/g\ DW\ plant}{\mu g/g\ soil})$	$Br_{rootveg}$ value was calculated by multiplying the uptake slope factor with a conversion factor of 2 x 10^9 g/ha soil. The uptake slope factor and the conversion factor were obtained from U.S. EPA (1992b) for root vegetables.	B-2-10	4.40E-02
Br_{ag} (fruit) $(\frac{\mu g/g\ DW\ plant}{\mu g/g\ soil})$	$Br_{root\ veg}$ value was calculated by multiplying the uptake slope factor with a conversion factor of 2 x 10^9 g/ha soil. The uptake slope factor and the conversion factor were obtained from U.S. EPA (1992b) for garden fruits.	B-2-9	4.60E-02
Br_{ag} (veg) $(\frac{\mu g/g\ DW\ plant}{\mu g/g\ soil})$	$Br_{root\ veg}$ value was calculated by weighting the uptake slope factors for garden fruits (75%) and leafy vegetables (25%) and multiplying the result with a conversion factor of 2 x 10^9 g/ha soil. The uptake slope factors and the conversion factor were obtained from U.S. EPA (1992b).	B-3-9	9.70E-02
Br_{forage} $(\frac{\mu g/g\ DW\ plant}{\mu g/g\ soil})$	$Br_{root\ veg}$ value was calculated by multiplying the uptake slope factor with a conversion factor of 2 x 10^9 g/ha soil. The uptake slope factor and the conversion factor were obtained from U.S. EPA (1992b) for leafy vegetables.	B-3-9	2.50E-01
Br_{grain} $(\frac{\mu g/g\ DW\ plant}{\mu g/g\ soil})$	$Br_{root\ veg}$ value was calculated by multiplying the uptake slope factors with a conversion factor of 2 x 10^9 g/ha soil. The uptake slope factor and the conversion factor were obtained from U.S. EPA (1992b) for grains/cereals.	B-3-9	5.40E-02
Bv_{ag} $(\frac{\mu g/g\ DW\ plant}{\mu g/g\ air})$	Metals are assumed to not experience air-to-leaf transfer, as cited in U.S. EPA (1995b).	B-2-8	NA
Bv_{forage} $(\frac{\mu g/g\ DW\ plant}{\mu g/g\ air})$	Metals are assumed to not experience air-to-leaf transfer, as cited in U.S. EPA (1995b).	B-3-8	NA

TABLE A-3-204

CHEMICAL-SPECIFIC INPUTS FOR ZINC (7440-66-6)

Parameter	Reference and Explanation	Equations	Value
Biotransfer Factors for Animals			
Ba_{milk} (day/kg FW)	Ba_{milk} values were obtained from U.S. EPA (1995a) for cadmium, selenium, and zinc. Values were calculated by dividing uptake slopes, as cited in U.S. EPA (1992b; 1995a), by a daily consumption rate of 20 kilograms dry weight per day and converting the result to a wet weight basis assuming a 87% moisture content in milk.	B-3-11	3.25E-05
Ba_{beef} (day/kg FW)	Ba_{beef} values were obtained from U.S. EPA (1995a) for cadmium, selenium, and zinc. Values were calculated by dividing uptake slopes, as cited in U.S. EPA (1992b; 1995a), by a daily consumption rate of 20 kilograms dry weight per day and converting the result to a wet weight basis assuming a 70% moisture content in beef.	B-3-10	9.00E-05
Ba_{pork} (day/kg FW)	Ba_{pork} values were obtained from U.S. EPA (1995a) for cadmium, selenium, and zinc. Values were calculated by dividing uptake slopes, as cited in U.S. EPA (1992b; 1995a), by a daily consumption rate of 4.7 kilograms dry weight per day and converting the result to a wet weight basis assuming a 70% moisture content in pork.	B-3-12	1.28E-04
Ba_{egg} (day/kg FW)	Ba_{egg} values were obtained from U.S. EPA (1995a) for cadmium, selenium, and zinc. Values were calculated by dividing uptake slopes, as cited in U.S. EPA (1992b; 1995a), by a daily consumption rate of 0.2 kilograms dry weight per day and converting the result to a wet weight basis assuming a 75% moisture content in eggs.	B-3-13	8.75E-03
$Ba_{chicken}$ (day/kg FW)	$Ba_{chicken}$ values were obtained from U.S. EPA (1995a) for cadmium, selenium, and zinc. Values were calculated by dividing uptake slopes, as cited in U.S. EPA (1992b; 1995a), by a daily consumption rate of 0.2 kilograms dry weight per day and converting the result to a wet weight basis assuming a 75% moisture content in chicken.	B-3-14	8.75E-03
BCF_{fish} (L/kg FW tissue)	Geometric mean value obtained from various literature sources (see Appendix A3.4.).	B-4-26	6.54E+02
BAF_{fish} (L/kg FW)	--	B-4-27	NA
$BSAF_{fish}$ (unitless)	--	B-4-28	NA
Health Benchmarks			
RfD (mg/kg/day)	U.S. EPA (1997b)	C-1-8	3.0E-01
Oral CSF $(mg/kg/day)^{-1}$	--	C-1-7	ND
RfC (mg/m^3)	Calculated from *RfD* using an inhalation rate of 20 m^3/day and a human body weight of 70 kg.	C-2-3	1.1E+00
Inhalation URF $(\mu g/m^3)^{-1}$	--	C-2-1	ND
Inhalation CSF $(mg/kg/day)^{-1}$	--	C-2-2	ND

Note: NA = Not applicable; ND = No data available
All parameters are defined in list of FATE AND TRANSPORT PARAMETERS on page A-3-iii.